

REPORT WITH DESCRIPTION OF MITIGATION SERVICE

Deliverable title Report with description of mitigation service

Deliverable number

Revision

Status

Planned delivery date
Actual date of issue
Nature of deliverable

D4.2

Final

Final

90/06/2022

Report

Nature of deliverable Report
Lead partner TNO
Dissemination level PU (Public)

The research leading to these results has received funding from the European Union's Horizon 2020 Research and Innovation programmes under grant agreement No 870301



About this document

Work package in charge: WP4: Policy Strategy: Attribution of Air Pollution Sources and Analysis of Emission Reduction Strategies

Lead author:

The Netherlands Organisation for Applied Scientific Research (TNO), Renske Timmermans

Other contributing authors:

The Netherlands Organisation for Applied Scientific Research (TNO), Richard Kranenburg, Ruud Janssen

University Corporation for Atmospheric Research (UCAR), Gabriele Pfister, Rajesh Kumar Institute of Urban Safety and Environmental Science, Beijing Academy of Science and Technology (IUSE|BMILP), Mo Dan, Yali Tong, Kun Wang Beijing Computing Center (BCC), Qi Zuo, Tong Liu

Breezometer, Yvonne Boose

Internal reviewer(s):

1st reviewer: Nicolas Huneeus (UCL)

2nd reviewer: Cathy Li (MPG)

Contacts: aq-watch@mpimet.mpg.de

Visit us on: www.aq-watch.eu

Disclaimer: This material reflects only the authors view and the Commission is not responsible for any use that may be made of the information it contains.

Table of Content

1	Abstract /publishable summary		5
2	Conclusion & Results		5
3	Project objectives		5
4	Detailed report on the deliverable		7
4.1	General description of mitigation service		7
U	E Emissions CAMS-glob-ant v4.2 US NEI emissions Chinese MEIC emissions		7 8 8 9
L N S R	Particulate matter mitigation service with LOTOS-EUROS model Mitigation service method with LOTOS-EUROS System set-up Results Evaluation		9 10 11 13
4 4 4	CO mitigation service with WRF-Chem 4.4.1 WRF-Chem model 4.4.2 Mitigation service method with WRF 4.4.3 System set-up 4.4.4 Results 4.4.5 Evaluation	-Chem	22 22 23 24 25 26
4.5	Operational implementation of the AQ-WA	ATCH AQ mitigation tool	29
4 4 4	Local PM, NO ₂ and O ₃ mitigation service w 4.6.1 SIRANE model 4.6.2 Mitigation service method with SIRA 4.6.3 System set-up 4.6.4 Results 4.6.5 Evaluation 4.6.6 Operational implementation		30 30 31 32 33 34
4.7	Next steps and recommendations		34
5	References (Bibliography)		36
6	Dissemination and uptake		39
6.1	. Uptake by the targeted audience		39
6.2	This is how we are going to ensure the upt	ake of the deliverables by the targeted audience	39
7	Deliverable timeliness		39
8	Changes made and/or difficulties en	ncountered, if any	39
9	Sustainability		39

AQ-WATCH Deliverable

9.1	Lessons learnt: both positive and negative that can be drawn from the experiences of the work to date	39
9.2	Links built with other deliverables, WPs, and synergies created with other projects	39
10	Full track of dissemination activities	40
11	Full track of publications and IP	40
11.1	Peer reviewed articles	40
11.2	Publications in preparation OR submitted:	40
11.3	Intellectual property rights resulting from this deliverable:	40

1. Abstract /publishable summary

Within the AQ-WATCH project, an operational mitigation service has been set-up providing policy makers with a tool for the assessment of the efficiency of alternative actions to mitigate air pollution as well as the development of effective strategy options for air pollution abatement.

The mitigation service allows the user to reduce the emissions from pre-defined emission sources and then provides information on the resulting expected changes in air pollutant concentrations (nitrogen dioxide (NO_2), particulate matter (PM), ozone (O_3) or carbon monoxide (CO)).

The service has been set-up for all three focus regions in AQ-WATCH, namely the Colorado Northern Front Range in the USA, the region around Santiago de Chile and Cangzhou in China. The service is based on 3 different models: 1. The LOTOS-EUROS model (targeting $PM_{2.5}$, for Colorado and Santiago), 2. the WRF-Chem model (targeting CO for Colorado), and 3. The SIRANE model (targeting PM, NO_2 and O_3 for Xinhua District of Cangzhou). This report outlines the set-up of the mitigation service and the status of the service operation.

2. Conclusion & Results

With this deliverable we achieved the following results:

- Interactive operational service with identification of the impact of CO emission reductions from different sources on CO air pollution in the Colorado Northern Front Range over the past 6 weeks complimented by a forecast for the next 2 days.
- Interactive operational service with identification of the impact of emission reductions in the Industry, Road traffic, Residential Combustion and Agriculture sectors on PM air pollution in Santiago de Chile and the Colorado Northern Front Range over the past 6 weeks complimented by a forecast for the next 2 days.
- Interactive operational service with identification of the impact of emission reductions in the Industry, Road traffic, Residential Combustion sectors on PM, NO₂ and O₃ air pollution in Xinhua district, Cangzhou over the past 6 weeks complimented by a forecast for the next 24 hours.

3. Project objectives

This deliverable contributes directly and indirectly to the achievement of specific objectives indicated in section 1.1 of the Description of the Action:

Specific objectives of the project	Contribution of this deliverable?
[1] To design and produce new global and regional air pollution atlases	No
that include the climatological distribution of chemical pollutants	

complemented by quantities such as the diurnal and seasonal variations, air quality and related health indices, premature mortality exceedance frequency, long-term trends, etc. [2] To develop software packages with the capability to provide more accurate daily forecasts of air quality at the regional scale including tailored high-resolution fire smoke and wind-blown dust forecasts; downscaling of air quality forecasts to 2 km resolution in urban areas. [3] To develop a source apportionment service to mitigate air pollution and hence increase the life expectancy of the population in different regions of the world, with special focus on the role of agricultural sources of air pollution and the potentially important effects of fracking operations. [4] To develop a new tool-box that will be user-friendly and accessible to decision-makers to evaluate the efficiency of proposed mitigation measures in different industrial sectors on the resulting level of air pollutants in three different regions of the world. This will establish the basis for their wider adoption and generalization. [5] To co-design, co-produce and co-evaluate for the first time prototype products and services with prime users in three regions of the world chosen for their specific level of economic, social and environmental		
frequency, long-term trends, etc. [2] To develop software packages with the capability to provide more accurate daily forecasts of air quality at the regional scale including tailored high-resolution fire smoke and wind-blown dust forecasts; downscaling of air quality forecasts to 2 km resolution in urban areas. [3] To develop a source apportionment service to mitigate air pollution and hence increase the life expectancy of the population in different regions of the world, with special focus on the role of agricultural sources of air pollution and the potentially important effects of fracking operations. [4] To develop a new tool-box that will be user-friendly and accessible to decision-makers to evaluate the efficiency of proposed mitigation measures in different industrial sectors on the resulting level of air pollutants in three different regions of the world. This will establish the basis for their wider adoption and generalization. [5] To co-design, co-produce and co-evaluate for the first time prototype products and services with prime users in three regions of the world chosen for their specific level of economic, social and environmental		
[2] To develop software packages with the capability to provide more accurate daily forecasts of air quality at the regional scale including tailored high-resolution fire smoke and wind-blown dust forecasts; downscaling of air quality forecasts to 2 km resolution in urban areas. [3] To develop a source apportionment service to mitigate air pollution and hence increase the life expectancy of the population in different regions of the world, with special focus on the role of agricultural sources of air pollution and the potentially important effects of fracking operations. [4] To develop a new tool-box that will be user-friendly and accessible to decision-makers to evaluate the efficiency of proposed mitigation measures in different industrial sectors on the resulting level of air pollutants in three different regions of the world. This will establish the basis for their wider adoption and generalization. [5] To co-design, co-produce and co-evaluate for the first time prototype products and services with prime users in three regions of the world chosen for their specific level of economic, social and environmental	air quality and related health indices, premature mortality exceedance	
accurate daily forecasts of air quality at the regional scale including tailored high-resolution fire smoke and wind-blown dust forecasts; downscaling of air quality forecasts to 2 km resolution in urban areas. [3] To develop a source apportionment service to mitigate air pollution and hence increase the life expectancy of the population in different regions of the world, with special focus on the role of agricultural sources of air pollution and the potentially important effects of fracking operations. [4] To develop a new tool-box that will be user-friendly and accessible to decision-makers to evaluate the efficiency of proposed mitigation measures in different industrial sectors on the resulting level of air pollutants in three different regions of the world. This will establish the basis for their wider adoption and generalization. [5] To co-design, co-produce and co-evaluate for the first time prototype products and services with prime users in three regions of the world chosen for their specific level of economic, social and environmental	frequency, long-term trends, etc.	
tailored high-resolution fire smoke and wind-blown dust forecasts; downscaling of air quality forecasts to 2 km resolution in urban areas. [3] To develop a source apportionment service to mitigate air pollution and hence increase the life expectancy of the population in different regions of the world, with special focus on the role of agricultural sources of air pollution and the potentially important effects of fracking operations. [4] To develop a new tool-box that will be user-friendly and accessible to decision-makers to evaluate the efficiency of proposed mitigation measures in different industrial sectors on the resulting level of air pollutants in three different regions of the world. This will establish the basis for their wider adoption and generalization. [5] To co-design, co-produce and co-evaluate for the first time prototype products and services with prime users in three regions of the world chosen for their specific level of economic, social and environmental	[2] To develop software packages with the capability to provide more	No
downscaling of air quality forecasts to 2 km resolution in urban areas. [3] To develop a source apportionment service to mitigate air pollution and hence increase the life expectancy of the population in different regions of the world, with special focus on the role of agricultural sources of air pollution and the potentially important effects of fracking operations. [4] To develop a new tool-box that will be user-friendly and accessible to decision-makers to evaluate the efficiency of proposed mitigation measures in different industrial sectors on the resulting level of air pollutants in three different regions of the world. This will establish the basis for their wider adoption and generalization. [5] To co-design, co-produce and co-evaluate for the first time prototype products and services with prime users in three regions of the world chosen for their specific level of economic, social and environmental	accurate daily forecasts of air quality at the regional scale including	
[3] To develop a source apportionment service to mitigate air pollution and hence increase the life expectancy of the population in different regions of the world, with special focus on the role of agricultural sources of air pollution and the potentially important effects of fracking operations. [4] To develop a new tool-box that will be user-friendly and accessible to decision-makers to evaluate the efficiency of proposed mitigation measures in different industrial sectors on the resulting level of air pollutants in three different regions of the world. This will establish the basis for their wider adoption and generalization. [5] To co-design, co-produce and co-evaluate for the first time prototype products and services with prime users in three regions of the world chosen for their specific level of economic, social and environmental	tailored high-resolution fire smoke and wind-blown dust forecasts;	
hence increase the life expectancy of the population in different regions of the world, with special focus on the role of agricultural sources of air pollution and the potentially important effects of fracking operations. [4] To develop a new tool-box that will be user-friendly and accessible to decision-makers to evaluate the efficiency of proposed mitigation measures in different industrial sectors on the resulting level of air pollutants in three different regions of the world. This will establish the basis for their wider adoption and generalization. [5] To co-design, co-produce and co-evaluate for the first time prototype products and services with prime users in three regions of the world chosen for their specific level of economic, social and environmental	downscaling of air quality forecasts to 2 km resolution in urban areas.	
the world, with special focus on the role of agricultural sources of air pollution and the potentially important effects of fracking operations. [4] To develop a new tool-box that will be user-friendly and accessible to decision-makers to evaluate the efficiency of proposed mitigation measures in different industrial sectors on the resulting level of air pollutants in three different regions of the world. This will establish the basis for their wider adoption and generalization. [5] To co-design, co-produce and co-evaluate for the first time prototype products and services with prime users in three regions of the world chosen for their specific level of economic, social and environmental	[3] To develop a source apportionment service to mitigate air pollution and	No
pollution and the potentially important effects of fracking operations. [4] To develop a new tool-box that will be user-friendly and accessible to decision-makers to evaluate the efficiency of proposed mitigation measures in different industrial sectors on the resulting level of air pollutants in three different regions of the world. This will establish the basis for their wider adoption and generalization. [5] To co-design, co-produce and co-evaluate for the first time prototype products and services with prime users in three regions of the world chosen for their specific level of economic, social and environmental	hence increase the life expectancy of the population in different regions of	
[4] To develop a new tool-box that will be user-friendly and accessible to decision-makers to evaluate the efficiency of proposed mitigation measures in different industrial sectors on the resulting level of air pollutants in three different regions of the world. This will establish the basis for their wider adoption and generalization. [5] To co-design, co-produce and co-evaluate for the first time prototype products and services with prime users in three regions of the world chosen for their specific level of economic, social and environmental	the world, with special focus on the role of agricultural sources of air	
decision-makers to evaluate the efficiency of proposed mitigation measures in different industrial sectors on the resulting level of air pollutants in three different regions of the world. This will establish the basis for their wider adoption and generalization. [5] To co-design, co-produce and co-evaluate for the first time prototype products and services with prime users in three regions of the world chosen for their specific level of economic, social and environmental	pollution and the potentially important effects of fracking operations.	
measures in different industrial sectors on the resulting level of air pollutants in three different regions of the world. This will establish the basis for their wider adoption and generalization. [5] To co-design, co-produce and co-evaluate for the first time prototype products and services with prime users in three regions of the world chosen for their specific level of economic, social and environmental	[4] To develop a new tool-box that will be user-friendly and accessible to	Yes
pollutants in three different regions of the world. This will establish the basis for their wider adoption and generalization. [5] To co-design, co-produce and co-evaluate for the first time prototype products and services with prime users in three regions of the world chosen for their specific level of economic, social and environmental	decision-makers to evaluate the efficiency of proposed mitigation	
basis for their wider adoption and generalization. [5] To co-design, co-produce and co-evaluate for the first time prototype products and services with prime users in three regions of the world chosen for their specific level of economic, social and environmental	measures in different industrial sectors on the resulting level of air	
[5] To co-design, co-produce and co-evaluate for the first time prototype products and services with prime users in three regions of the world chosen for their specific level of economic, social and environmental	pollutants in three different regions of the world. This will establish the	
products and services with prime users in three regions of the world chosen for their specific level of economic, social and environmental	basis for their wider adoption and generalization.	
chosen for their specific level of economic, social and environmental	[5] To co-design, co-produce and co-evaluate for the first time prototype	Yes
·	products and services with prime users in three regions of the world	
dovoloment	chosen for their specific level of economic, social and environmental	
development.	development.	

This deliverable directly contributes to the achievement of specific objectives indicated in the description of the Work Package.

Objectives of WP4	Relevance in this deliverable?
4.1 To establish a user driven service for (NRT) source apportionment	No
information	
4.2 To establish a user driven service for mitigation information on	Yes
most effective emission reduction measures	
4.3 To establish a fracking service for the assessment of the impact of	No
fracking activities on air pollution	
4.4 To improve the quality of the above mentioned three services,	Yes
through validation, customization and targeted developments	

4. Detailed report on the deliverable

4.1 General description of mitigation service

Within the AQ-WATCH project, several services are set-up that provide information on the past, current and future (next 2-3 days) air quality situation in the world and prototypes are provided for the three target regions (Santiago de Chile, Colorado Northern Front Range and Xinhua district of Cangzhou). The aim of this service is to go a step further by providing insight in the potential impact of emission reductions for specific sources. This information is crucial to support the design of effective mitigation strategies for improving air quality, and hence public health in the target regions.

Three different air quality models and techniques are applied to provide the information on mitigation potential for the three target regions: Santiago de Chile, the Colorado Northern Front Range in USA and Cangzhou in China. The models and the systems used for the mitigation service are described in Sections 4.3, 4.5 and 4.4, including maps of target regions. The systems are in general transferable to any other region, with the side note that the quality of the results is depending on the quality of the available information used as input to the systems, e.g. emissions and their distribution in time and space, meteorological data and land use information. Therefore, the set-up of the systems needs to be evaluated for any new region where it is applied to.

The regions and species targeted by each of the models/systems are summarised in **Table 1**.

	South America- Chile- Santiago	CONUS- Colorado Northern Front Range	China - Xinhua district of Cangzhou
LOTOS-EUROS	PM	PM	
WRF-Chem	СО	СО	
SIRANET			PM, NO ₂ and O ₃

Table 1: Overview of models used, and regions and species targeted by current operational mitigation service

In the following sections, the emission input and set-up of the source apportionment systems are presented.

4.2 Emissions

The source attribution services are based on chemistry transport models which are dependent on emission information from different sources within the domains of interest. Below we provide short descriptions of the different emission inventories used within the service.

CAMS-glob-ant v4.2

The CAMS global anthropogenic emissions (Granier et al., 2019) are based on the EDGARv4.3.2 inventory developed by the European Joint Center (JRC, Crippa et al., 2018) and the CEDS emissions (Hoesly et al., 2018), which provide historical emissions for the 6th IPCC Assessment Report (AR6). The inventory contains emission data for 12 different sectors. Monthly emission profiles provided by CAMS-GLOB-TEMPO (Granier et al., 2019) are applied to the annual emissions from EDGARv4.3.2 for the years 2000-2012. After 2012, the data are linearly extrapolated to 2020 using trends derived from the CEDS emissions for the years 2011-2014. Note that the emissions do not incorporate the impact of the COVID pandemic on the emissions yet, since this dataset became available in spring 2020. The weekly and hourly emission profiles must be supplied by the model itself.

US NEI emissions

The National Emissions Inventory (NEI) is a detailed inventory including estimated emission numbers for criteria pollutants and hazardous air pollutants. The NEI is released every three years based primarily upon data provided by State, Local, and Tribal air agencies for sources in their jurisdictions and supplemented by data developed by the US EPA. The NEI is built using the Emissions Inventory System (EIS) first to collect the data from State, Local, and Tribal air agencies and then to blend that data with other data sources.

The U.S. National Emission Inventory (NEI) 2017, which provides speciated gas phase and aerosol emissions for 2017 has become available in 2020. Information on the inventory including technical documentation, reports and summaries is available from the U.S. EPA website (https://www.epa.gov/air-emissions-inventories/2017-national-emissions-inventory-nei-data).

Typically, the use of NEI emissions requires running the complex Sparse Matrix Operator Kernel Emissions (SMOKE) tool which generates emissions in a format for use in the Community Multiscale Air Quality (CMAQ) model. Through collaborations between UCAR and U.S. EPA, the NEI 2017 has been made available in CMAQ-ready netCDF format at 12 x 12 km² resolution over the contiguous U.S. and can be download from the UCAR NCAR/ACOM WRF-Chem webpage (https://www2.acom.ucar.edu/wrf-chem/wrf-chem-tools-community). The provided emissions are day and year-specific with hourly resolution. Sector specific information is available for major source categories. Chemical speciation follows the Carbon Bond mechanism version 6 (CB6). NCAR/ACOM also provides a tool which transforms the CMAQ ready files into a format for use in WRF-Chem. Since the NEI emissions have day of the week variability, we have developed a mapping to conserve the day of week when using NEI 2017 emissions for other years (e.g., 2021). In this mapping, the first Monday of 2017 is mapped to the first Monday of the target year and so on.

Chinese MEIC emissions

The Multi-resolution Emission Inventory for China (MEIC) contains detailed emission information for anthropogenic air pollutants in China. The inventory is developed and maintained by Tsinghua University since 2010 (http://meicmodel.org/). It provides emission data for 10 major air pollutants from more than 700 anthropogenic sources in China from 1990 to present. For the model chain, that is used in the mitigation service in China, a modified version of the MEIC 2017 regional emission inventory is used at 0.25 degree resolution, where the industrial emissions are replaced with regional scale emission data for 2020 generated by IUSE (Wang et al., 2022). In the local scale model SIRANE, only emissions for road traffic, residential and industry sector are used. These emissions for the Xinhua district in Cangzhou have been obtained through downscaling the 2017 road traffic and the residential sector emissions from MEIC to a finer grid with 10 meter resolution by using population distributions data, road network and building distribution map as proxies and for the industry sector emissions for the year 2020 as mentioned above have been used. The emission data process followed the guidance for emission setting method of SIRANE (http://air.ec-lyon.fr/SIRANE/index.php?Lang=EN).

4.3 Particulate matter mitigation service with LOTOS-EUROS

LOTOS-EUROS model

The 3-D regional chemistry transport model LOTOS-EUROS aims to simulate air pollution in the lower troposphere. Meteorological input is obtained from an off-line model, in this case from ECMWF Integrated Forecasting System (IFS) (Flemming et al., 2015).. The model is of intermediate complexity in the sense that the relevant processes are parameterized in such a way that the computational demands are modest, enabling long-term simulations within acceptable computational time. LOTOS-EUROS version 2.2 was used for the AQ-WATCH forecasts. For a more detailed model description more details of the model please refer to Manders et al. (2017) and the website www.lotos-euros.tno.nl.

The model is a Eulerian grid model, which means that the calculations are performed on a fixed three-dimensional grid. On this grid the concentration changes due to advection, vertical mixing, chemical transformations and removal by wet and dry deposition are performed. For the chemistry schemes, the model adopts the CBM4 scheme for calculation of gas-phase chemistry (Gery et al., 1989). For secondary inorganic chemistry Isorropia II (Fountoukis and Nenes, 2007) is used and the formation of coarse nitrate and ammonium sulphate through heterogeneous chemistry on wet aerosol surfaces follows Wichink Kruit et al. (2012). In cloud oxidation processes are described in a pH-dependent cloud chemistry scheme (Banzhaf et al., 2012). Land use information is obtained from the Global Land Cover (GLC) 2000 database (http://forobs.jrc.ec.europa.eu/products/glc2000/glc2000.php). The boundary layer height is taken from input meteorology from ECMWF.

For dry deposition, a resistance approach is used, as implemented in the DEPAC (DEPosition of Acidifying Compounds) module (Van Zanten et al., 2010). Furthermore, a compensation point approach for ammonia is included in the dry deposition module (Wichink Kruit et al., 2012). The deposition scheme by Zhang (2001) is used for particles, explicitly including particle size and sedimentation. The wet deposition module considers in/below-cloud scavenging and accounts for droplet saturation (Banzhaf et al., 2012).

The process calculations require information about anthropogenic emissions and meteorological conditions, which must be prescribed to the model system. For anthropogenic emissions in the operational service, the CAMS-GLOB-ANT v4.2 is used (Granier et al., 2019) (see section 0). Dust and sea salt aerosol emissions are calculated online. The MEGANv2 dataset is adopted for biogenic emissions (Guenther et al., 2012) and the GFAS wild fire product is used for biomass burning (Kaiser et al., 2012). Default diurnal and weekly profiles (made available with the CAMS regional emission dataset) are applied to the emission data by sector. Note that these time profiles originate from European studies and may not be fully representative for the two targeted regions within AQ-WATCH. Previous forecast results are adopted for the initial conditions of forecast runs, while ECMWF IFS data are used as the boundary conditions (Flemming et al., 2015).

Mitigation service method with LOTOS-EUROS

The mitigation service for $PM_{2.5}$ with the LOTOS-EUROS model is based on the same method as used in the CAMS-Air Control Box (ACT) tool for Europe (Colette et al., 2022). In this method, the concentration change due to an emission reduction is represented by a surrogate model, which emulates the behavior of a CTM over a broad range of emission reductions.

This surrogate model consists of a second order polynomial function for each sector that we include in the mitigation tool: agriculture (AGR), industry (IND), road traffic (TRA) and residential heating (RES). In addition, interaction terms are added that account for the fact that simultaneous emission reductions in more than one sector lead to concentration reductions that are not simply the sum of the reductions from the individual sectors.

The full equation of the surrogate model is as follows:

$$\begin{split} &C_{ctrl} - C_{scen} = \\ &\alpha_{agr} \cdot \left(R_{agr} \cdot E_{ctrl,agr}\right) + \beta_{agr} \cdot \left(R_{agr} \cdot E_{ctrl,agr}\right)^2 + \\ &\alpha_{ind} \cdot \left(R_{ind} \cdot E_{ctrl,ind}\right) + \beta_{ind} \cdot \left(R_{ind} \cdot E_{ctrl,ind}\right)^2 + \\ &\alpha_{tra} \cdot \left(R_{tra} \cdot E_{ctrl,tra}\right) + \beta_{tra} \cdot \left(R_{tra} \cdot E_{ctrl,tra}\right)^2 + \\ &\alpha_{res} \cdot \left(R_{res} \cdot E_{ctrl,res}\right) + \\ &\gamma_{agr,ind} \cdot \left(R_{agr} \cdot E_{ctrl,agr}\right) \cdot \left(R_{ind} \cdot E_{ctrl,ind}\right) + \\ &\gamma_{agr,tra} \cdot \left(R_{agr} \cdot E_{ctrl,agr}\right) \cdot \left(R_{tra} \cdot E_{ctrl,tra}\right) + \\ &\gamma_{tra,ind} \cdot \left(R_{tra} \cdot E_{ctrl,tra}\right) \cdot \left(R_{ind} \cdot E_{ctrl,ind}\right) \end{split}$$

, where C_{ctrl} is the concentration of the species in the control run and C_{scen} the concentration for a certain emission reduction scenario in which emissions of one or more sectors are reduced. Other parameters are as follows:

AQ-WATCH Deliverable

 α_{sect} : sector-specific coefficient of polynomial ($\mu g \ m^{-3} \ kTon^{-1} \ day^{-1}$)

β_{sect}: sector-specific coefficient of polynomial (μg m⁻³ kTon⁻² day⁻²)

 R_{sect} : sector-specific emission reduction factor (unitless); allowed range (0,1)

E_{ctrl,sect}: total emission of tracer (precursor) for a specific sector in the control run (kTon day⁻¹)

γ_{sect1,sect2}: interaction term between sector 1 and sector 2 (μg m⁻³ day² kTon⁻²)

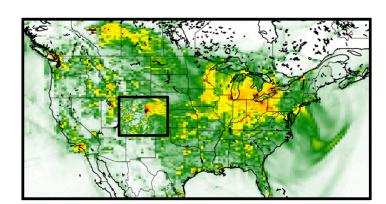
Note that for the sector residential heating, Colette et al. (2022) found that the response of concentrations to emission reductions is sufficiently linear, probably because this source is mostly associated with primary PM components which do not react chemically in the atmosphere, so the polynomial can be reduced to a linear relationship and no interaction terms with other sectors are needed.

The coefficients in this surrogate model are obtained by fitting the model to a set of LOTOS-EUROS runs in which emission reduction scenarios have been applied (the brute force runs). This set of runs is the same as in Colette et al. (2022) and contains emission reductions for single and for multiple sectors over a wide range of emission reductions, in addition to a control run. In this choice of brute force runs, we implicitly assume that the set of simulations that was found to accurately describe the concentration response to emission reductions over Europe also will perform well when applied to North- and South-America. We have evaluated this assumption by running an additional set of brute force runs for two selected periods and comparing the performance of the surrogate model against these independent test runs. The setup of the LOTOS-EUROS simulations and the surrogate model is described in more detail in the following paragraphs. This set-up is flexible and may be changed based on user consultations.

Further, the surrogate model is currently designed for emission reductions that are applied over the large continental scale domain simultaneously, see next paragraph for specifications.

System set-up

The LOTOS-EUROS model is run for the North- and South American domains with the following specifications. For the target region in Colorado Northern Front Range in the US, two domains (see Figure 1 left plot) are set up: An outer domain $(25^{\circ}-55^{\circ}\text{N}\;;60^{\circ}-130^{\circ}\text{ W})$ which is run first at a resolution of $0.5^{\circ}\times0.25^{\circ}$ (or 36/50 km \times 28 km), and an inner domain $(36^{\circ}-42^{\circ}\text{ N}\;;110^{\circ}-101^{\circ}\text{ W})$ which is then nested within the outer domain and run at a resolution of $0.1^{\circ}\times0.05^{\circ}$ (or 8 km \times 6 km). Both model runs are performed with 12 levels vertically. For the target region of Santiago de Chile in South America (see Figure 1 right plot) three domains are set up through a similar one-way nesting procedure, with the horizontal resolutions of the outermost to the innermost inner domain $(35^{\circ}-32^{\circ}\text{ S}\;;72^{\circ}-69^{\circ}\text{ W})$ equal to $0.5^{\circ}\times0.25^{\circ}$ (or 33/54 km \times 28 km), $0.25^{\circ}\times0.125^{\circ}$ (or 21/26 km \times 14 km) and $0.05^{\circ}\times0.025^{\circ}$ (or 3 km \times 3 km) respectively, and all domains with 12 levels vertically.



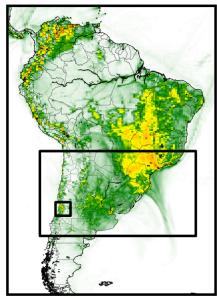


Figure 1: The two North American domains with zoom over Colorado Northern Front Range (left) and three South American domains with zoom over South America, Chile and Santiago (right) of the LOTOS-EUROS-TNO model

For both regions, we applied the CAMS-GLOB-ANT v4.2 emissions as described in Section 0. For each domain, 12 simulations are run, including a control run and several brute force runs with emission reductions. The 11 emission reduction scenarios that we used to fit the surrogate model are shown in Table 2. Here agriculture includes the CAMS-GLOB-ANT sectors agriculture livestock (agl), Agriculture soils (ags) and Agriculture waste burning (awb). All pollutant emissions within one sector are reduced with the same percentage. Note that as stated before for residential combustion, the response of concentrations to emission reductions is nearly linear, so we have implemented a linear relationship for which we only need 1 reduction run (RES90 in Table 2) and no interaction terms with other sectors are needed.

Scenario	Sectors	Reductions (%)
AGR60	Agriculture	60
AGR100	Agriculture	100
IND60	Industrial processes	60
IND100	Industrial processes	100
TRA60	Road transportation	60
TRA100	Road transportation	100
RES90	Residential/commercial heating combustion	90
	(heating, cooking and other	
	small scale combustion)	
	(res)	

AGR30_IND60	Agriculture, Industrial	30, 60	
	processes		
TRA100_AGR100	Road Traffic, Industrial	100, 100	
	processes		
TRA30_IND60	Road Traffic, Industrial	30, 60	
	processes		
AGR100_IND100_RES100_TRA100	Agriculture, Industrial	100, 100, 100, 100	
	processes, residential and		
	other small scale		
	combustion, road		
	transportation		

Table 2: set of emission reduction scenarios that is used to fit the surrogate model

For the operational service, the set of 12 LOTOS-EUROS simulations is run daily for the previous and the current day. The coefficients of the surrogate model are then obtained by fitting the equation provided in section 0 to the output of these runs.

With this set-up, the service presents concentration changes due to emission changes in the entire large domain (South America or continental US). If required by users the set-up could be adapted to include changes for a specific country or state only.

Results

Figure 2 shows an example of the results from the mitigation tool for the Santiago de Chile region. The figure reflects the results if the user would choose an emission reduction of 20% in agricultural emissions and 50% in road traffic emissions. It is clear that such emission reductions will lead to a decrease in $PM_{2.5}$ concentrations over the entire domain with values up to several $\mu g \ m^{-3}$. As expected, the changes are largest over the populated areas with dense road network. The delta figure allows the user to evaluate whether a specific mitigation measure has the desired impact on pollutant concentrations.

The results shown here are for one specific day, but will be made available through the interface for the past 6 weeks, today and the upcoming 2 days.

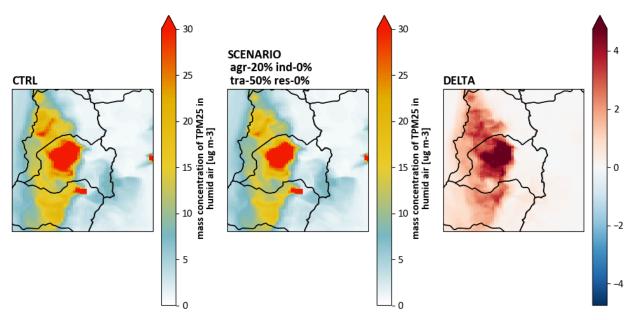


Figure 2: example results from the mitigation tool: PM_{2.5} concentrations over the Santiago domain for the control and the TRA50_AGR20 scenario and the difference between them for July 1st, 2016.

Evaluation

To evaluate the performance of the surrogate model to predict air pollution changes, we have performed an evaluation, consisting of comparing the surrogate model with a set of brute force reduction runs with LOTOS-EUROS (Table 3) which were not included in the fitting procedure. We made sure to include several scenarios that involve agriculture, since this is a sector which is associated with non-linearities in the emission-concentration relationship for PM, due to the large NH_3 emissions from this sector and the role that NH_3 plays in the formation of secondary inorganic aerosols. We also included some scenarios with simultaneous reductions in the agriculture and road traffic sectors because of the interaction between these two sources (agriculture mostly providing NH_3 and road traffic mostly providing NO_2) during the formation of the $PM_{2.5}$ component NH_4NO_3 . We performed this evaluation for Santiago and for Colorado for the months of January and July 2016, to be sure to include both a summer and a winter month in both regions.

Scenario	Sectors	Reductions (%)
AGR10	Agriculture	10
AGR30	Agriculture	30
AGR90	Agriculture	90
TRA60_AGR30	Road Traffic, Agriculture	60, 30
TRA30_AGR60	Road Traffic, Agriculture	30, 60

Table 3: set of emission reduction scenarios that is used to evaluate the surrogate model

Santiago

We have run LOTOS-EUROS with these emission scenarios over the Santiago domain. For each of the scenarios (Table 3) and in both summer and winter, the median error was well below 1% (Figure 3). 95% of locations/times showed a relative error below a few percent, however, for a few individual grid cells and days in all scenarios, the error exceeded 10%.

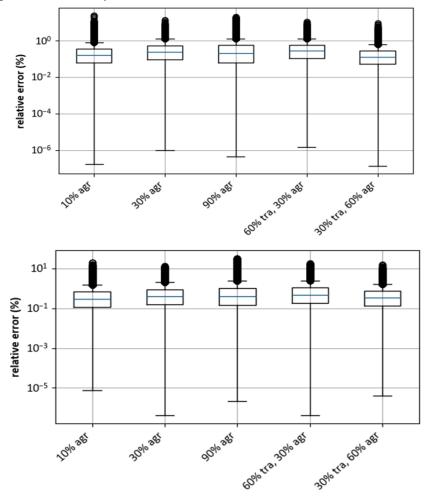


Figure 3: daily values of the relative error between the surrogate model and LOTOS-EUROS for each grid cell in the Santiago domain for 5 emission reduction scenarios in January 2016 (top) and July 2016 (bottom). Blue lines indicate the median, boxes indicate the lower and upper quartiles (25 and 75 percentiles). The horizontal black lines indicate 1.5x the inter-quartile range (defined as the range between the 25 and 75 percentile) and the circles near the top indicate single outliers.

We had a closer look at the scenario which showed the highest median error: the TRA60_AGR30 scenario. For the January 2016 period (Figure 4) the domain averaged time series showed very good agreement between the surrogate model and the brute force runs from LOTOS-EUROS,

which is also reflected in the scatter plot ($r^2=1.0$, mean relative error=0.44%). Also the monthly mean concentration fields were very similar.

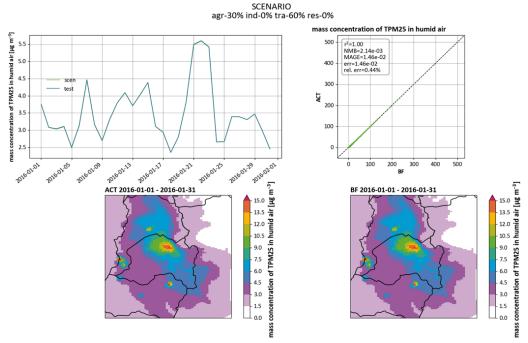


Figure 4: domain average time series (upper left), daily scatter plot for all grid cells (upper right) and monthly mean concentration maps of PM_{2.5} in the TRA60_AGR30 scenario for January 2016. Maps include the surrogate model (bottom left) and the LOTOS-EUROS brute force (BF, bottom right) simulation results.

In addition, maps of the absolute and relative error (Figure 5) show that the surrogate model reproduced the response in the Santiago area well, while the largest errors were found in the mountains to the east of Santiago and in an area to the Northwest of the city. The maximum monthly mean relative error in a single grid cell was about 2%.

For the July 2016 period, we found similar results. The surrogate model reproduced the domain averaged time series and the monthly mean concentration map well (Figure 6), although the error was a bit higher in the worst-performing scenario compared to January 2016 (mean relative error=0.94%). When we looked at the spatial distribution of the errors, we found (Figure 7) that these show the highest absolute values over the western half of the domain, including the Santiago area. However, the relative error was quite low over Santiago, so the higher relative errors were not associated with the highest concentrations. Instead, they showed maxima in the area to the west of Santiago and in the mountains to the east.

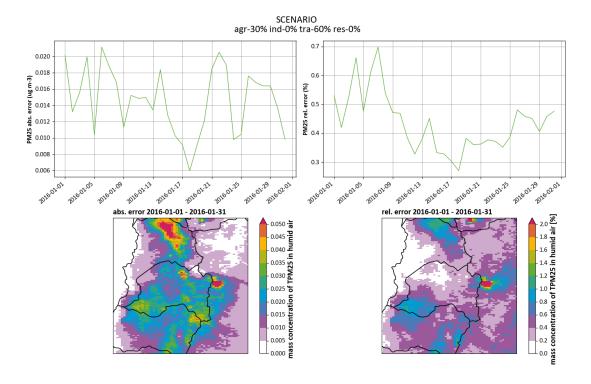


Figure 5: domain average time series and monthly mean maps of the absolute and relative error of PM_{2.5} in the TRA60_AGR30 scenario for January 2016.

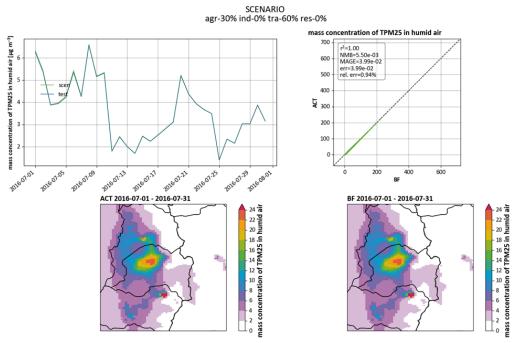


Figure 6: domain average time series (upper left), daily scatter plot for all grid cells (upper right) and monthly mean concentration maps of $PM_{2.5}$ in the TRA60_AGR30 scenario for July 2016. Maps include the surrogate model

(bottom left) and the LOTOS-EUROS brute force (BF, bottom right) simulation results.

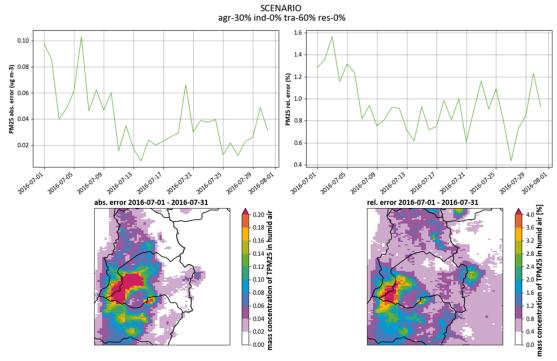


Figure 7: domain average time series and monthly mean maps of the absolute and relative error of $PM_{2.5}$ in the TRA60_AGR30 scenario for July 2016.

From the evaluation, we conclude that the surrogate model performed well for the tested scenarios over the domain as a whole. The surrogate model had some more difficulties in specific grid cells, however these seem to be outside of the main region of interest with highest PM concentrations.

Colorado

For Colorado, we also found median errors well below 1% for all scenarios in both periods and below a few percent for 95% of all locations/times (Figure 8), which shows that the surrogate model performed well for this domain too. Only for individual grid cells on single days, the error was above 10%.

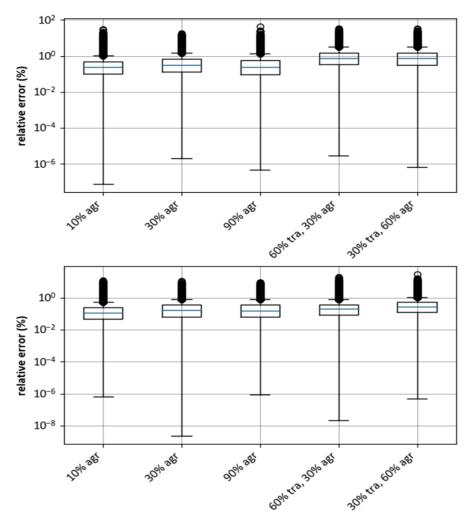


Figure 8: Daily values of the relative error between the surrogate model and LOTOS-EUROS for each grid cell in the Colorado domain for 5 emission reduction scenarios in January 2016 (top) and July 2016 (bottom). Blue lines indicate the median, boxes indicate the lower and upper quartiles (25 and 75 percentiles). The horizontal black lines indicate 1.5x the inter-quartile range (defined as the range between the 25 and 75 percentile) and the circles near the top indicate single outliers.

We took a closer look at the worst performing scenarios for Colorado for both the winter and the summer period. In the winter period, for this scenario the modeled PM_{2.5} concentrations over Colorado were generally low. Some of the highest concentrations were found in the northern Colorado front range. The surrogate model was able to reproduce the mean concentration fields and the trends for this period in the TRA60_AGR30 scenario (Figure 9). The mean relative error was just above 1%.

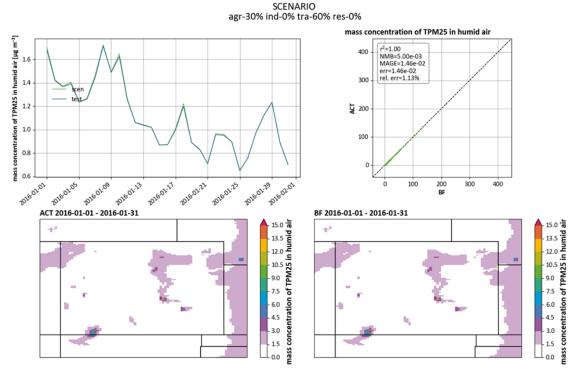


Figure 9: domain average time series (upper left), daily scatter plot for all grid cells (upper right) and monthly mean concentration maps of PM_{2.5} in the TRA60_AGR30 scenario for January 2016. Maps include the surrogate model (bottom left) and the LOTOS-EUROS brute force (BF, bottom right) simulation results.

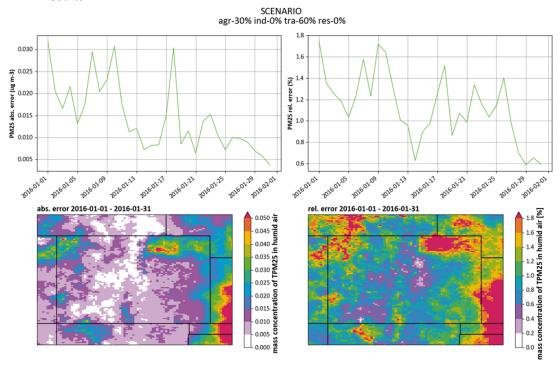


Figure 10: domain average time series and monthly mean maps of the absolute and relative error of PM_{2.5} in the TRA60_AGR30 scenario for January 2016.

The highest absolute errors for this scenario were found in the southeastern corner of the domain, outside the state of Colorado (Figure 10). Another area with high errors was found in the northeastern corner of Colorado state, but also here errors were not associated with the highest peaks in the modelled PM_{2.5} concentrations. In the Northern Colorado Front Range area the relative errors were small.

For the summer period (July 2016), the TRA30_AGR60 scenario showed the worst performance as measured by the median relative error (Figure 8). The modelled PM_{2.5} showed peak concentrations in specific locations due to wildfires, but the mean relative error in the scenario was well below 1% (Figure 11).

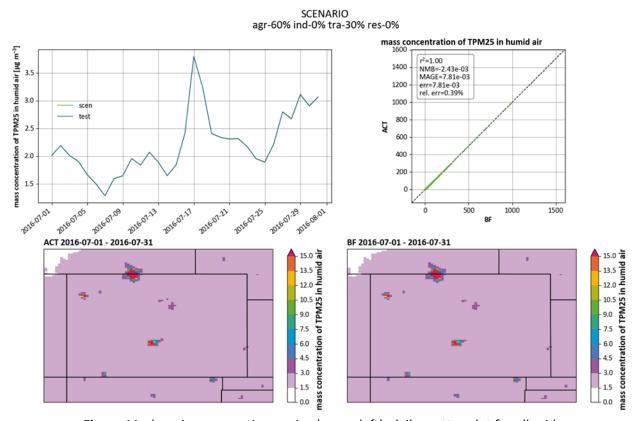


Figure 11: domain average time series (upper left), daily scatter plot for all grid cells (uppe right) and monthly mean concentration maps of PM_{2.5} in the TRA30_AGR60 scenario for July 2016. Maps include the surrogate model (bottom left) and the LOTOS-EUROS brute force (BF, bottom right) simulation results.

The maps of the absolute and relative error confirmed the good performance of the surrogate model even for the worst-performing scenario (Figure 12). An East-to-west gradient was visible in the absolute and relative error, but the latter was below 1% at all locations.

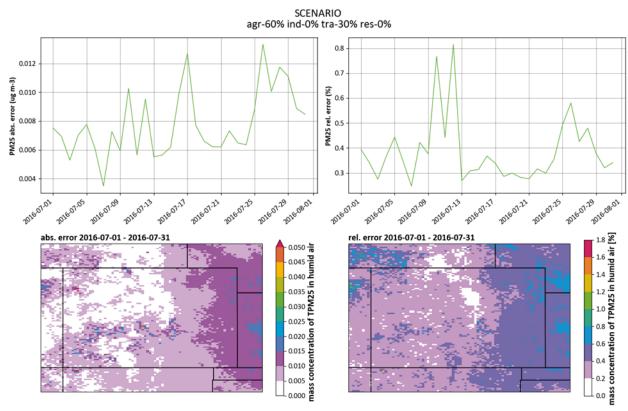


Figure 12: domain average time series and monthly mean maps of the absolute and relative error of PM_{2.5} in the TRA30_AGR60 scenario for July 2016.

4.4 CO mitigation service with WRF-Chem

WRF-Chem model

The Weather Research and Forecasting model with Chemistry (WRF-Chem) is a publicly available community model (Grell et al., 2005; Powers et al., 2017). The chemistry component of WRF-Chem is fully consistent with the meteorological component; both components use the same transport scheme (mass and scalar preserving), the same horizontal and vertical grids, the same physical schemes for sub grid-scale transport, and the same time step for transport and vertical mixing.

UCAR is the main developer of the WRF model and a major contributor to WRF-Chem (https://www2.acom.ucar.edu/wrf-chem). WRF-Chem is a fully coupled regional chemical transport model which offers a wide range of chemical and physical options. Based on WRF-Chem V3.9.1, UCAR has setup a regional forecast system over the contiguous U.S. (CONUS) at 12 km x

12 km which has been in operation since May 2019. A second forecast system based on WRF-Chem V4.1 for AQ-WATCH has been added in June 2020 (Section 0). The forecast products and near-real time evaluation results are visualized on a dissemination website (https://www.acom.ucar.edu/firex-aq/forecast.shtml). These forecasts serve as input to the AQ-WATCH attribution and mitigation service.

Mitigation service method with WRF-Chem

In the model setup, six CO tracers are setup that are used to track (1) CO emitted from anthropogenic and (2) biomass burning emissions inside the model domain that covers the contiguous United States (CONUS), (3) CO produced from the photochemical oxidation of VOCs, (4) background CO generated from the sources located outside of the CONUS and (5) for sources in Asia only, and (6) background CO generated from fires outside of CONUS. Information on the non-CONUS tracers is taken from the UCAR Whole Atmosphere Community Climate Model (WACCM) forecasts. The CO tracers do not affect the model physics or chemistry but undergo all model processes (Kumar et al., 2021). Key meteorological parameters, air pollutants and CO tracers are displayed on the UCAR dissemination forecast webpage.

Since atmospheric CO does not have any reservoir species as it is primarily lost through direction reaction with the hydroxyl (OH) radical, the linear assumption works well for source attribution of CO. Linear assumption means that total CO in the model becomes equal to the sum of source-specific CO tracers after the spin up period has passed. Please refer to section 0 for an evaluation of this assumption.

Since our AQ-WATCH forecasting system for Colorado started on 01 June 2020, the tracer contributions can be used for mitigation services starting in July 2020 assuming a similar 1-month spin up time for CO tracers in the AQ-WATCH set up.

The equation which is used in the mitigation service for CO is:

$$C_{scen} = C_{ctrl} - C_{tr1} \cdot R_{tr1} - C_{tr2} \cdot R_{tr2} - C_{tr3} \cdot R_{tr3} - C_{tr4} \cdot R_{tr4}$$

, where C_{ctrl} is the concentration of the species in the control run and C_{scen} the concentration for a certain emission reduction scenario in which emissions of one or more sources are reduced. Other parameters are as follows:

 C_{tr} : tracer-specific contribution ($\mu g \ m^{-3}$) for each of the 4 sources targeted in the mitigation service

R_{tr}: tracer/source-specific emission reduction factor (unitless); allowed range from 0 to 1 The four targeted sources in the CO mitigation service are:

- (1) CO emitted from all anthropogenic sources together inside the model domain that covers the contiguous United States (CONUS)
- (2) biomass burning emissions inside the model domain that covers the contiguous United States (CONUS)
- (3) CO produced from the photochemical oxidation of VOCs

(4) background CO generated from the sources located outside of the CONUS

System set-up

The source attribution and mitigation services for CO are based on the AQ-WATCH forecasts. The configuration for the AQ-WATCH forecast setup, which has been running in parallel to the standard setup since June 2020, covers the CONUS at 12 km x 12 km and Colorado at 4 km x 4 km grid spacing. Gas-phase chemistry is simulated with the T1 MOZART scheme (Emmons et al., 2020) that is coupled to the Goddard Global Ozone Chemistry Aerosol Radiation and Transport (GOCART) aerosol scheme (Chin et al., 2000; Ginoux et al., 2001). For more details on the overall model setup we refer to https://www.acom.ucar.edu/firex-aq/tracers.shtml and to Kumar et al. (2021). The boundary layer is simulated using the YSU scheme and land use information is provided by MODIS products (https://lpdaac.usgs.gov). A resistance-based approach is adopted to simulate dry deposition (Wesely, 1989), while in-cloud and below-cloud scavenging is included for wet deposition (Neu and Prather, 2012).

The WRF-Chem-UCAR model forecasts are initialized daily and forced at the lateral boundaries by 3-hourly meteorological analysis data from the NCEP Global Forecast System (GFS) at 0.25° x 0.25° resolution (https://rda.ucar.edu/datasets/ds084.1/). For anthropogenic emissions, the National Emission Inventory (NEI) 2017 at a 12 km resolution is used for the AQ-WATCH setup (as described in Section 4.2), which is regridded to the model resolution using a mass conserving mapping. Day of week mapping from the NEI representative year to the target year is applied to the emission data, and diurnal variations based on activity data as well as standard emission profiles are included for all sectors. For the other emission inputs, the GOCART module is adopted for online calculation of the emissions of dust and sea-salt aerosols (Chin et al., 2000; Ginoux et al., 2001), MEGANv2 for biogenic emissions (Guenther et al., 2012), and FINNv1 for biomass burning (Wiedinmyer et al., 2011). The latter is subject to an online plume rise parametrization (Freitas et al., 2007). Dynamic 6-hourly outputs from UCAR's WACCM forecast system (https://www.acom.ucar.edu/waccm/forecast/) are adopted as the boundary conditions of chemical variables. WACCM simulations also provide oxygen and ozone column densities used for photolysis calculations (Marsh et al., 2013). Figure 13 provides a schematic of the forecast system. Forecasts are issued daily for the next 2 days.

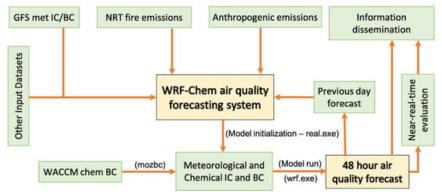


Figure 13: Architecture of the UCAR air quality forecasting system (from Kumar et al., 2021)

Results

Figure 14 shows an example of the hourly CO source attribution information averaged over the Colorado Front Range monitoring sites that can inform mitigation strategies. Anthropogenic CO emissions and inflow from the lateral domain boundaries (which includes the CO from Asia, CO from fires outside CONUS and other sources outside CONUS) are clearly the largest contributors to surface CO mixing ratios in the Colorado Front Range. A significant contribution to the CO inflow comes from the emissions in Asia particularly during November to April. Fires outside the CONUS contribute more than photochemical productions from the non-methane volatile organic compounds and the CONUS fires during November to April. The relative contribution of photochemistry and CONUS fires is the highest during June to September but overall, still fairly low compared to anthropogenic emissions and inflow. The contribution of fires to the CO in WRF-Chem may be biased low because of a known underestimation of biomass burning emissions by the Fire Inventory from NCAR, which should be improved when switching to an updated fire emissions inventory which is planned for the near future. Similar information is produced for each 48-h forecast cycle and is in the process of integration in the AQ-WATCH toolkit.

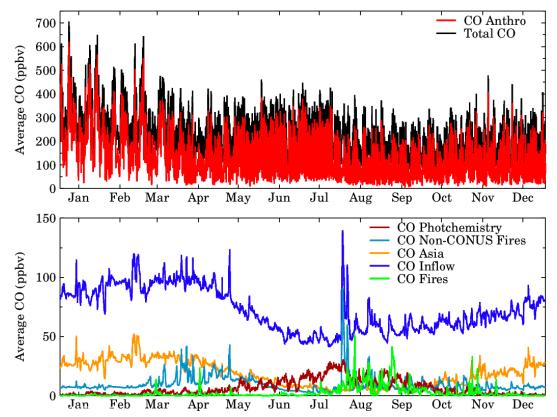


Figure 14: time series of hourly total CO mixing ratios (black in top plot) averaged over the Colorado front range monitoring sites in 2021 along with the CO mixing ratios from anthropogenic emissions (red, in top plot), background CO inflow from the lateral domain boundaries (blue), fires within the CONUS (green), fires outside the CONUS (teal), and CO emissions from Asia (orange).

Evaluation

The performance of the CO mitigation service is depending on the ability of the underlying WRF-Chem model to correctly represent different source contributions of CO. An evaluation of the WRF-Chem CO values with MOPITT satellite observations showed that WRF-Chem captures the variations in the vertical profiles of MOPITT retrieved CO with higher values near the surface and a secondary peak in the upper troposphere but underestimates the MOPITT retrieved CO profiles throughout the troposphere (Figure 15). It is well known that global models significantly underestimate tropospheric CO (Emmons et al., 2020). Thus, some of the underestimation can be attributed to errors in inflow of CO from the global model input into our model domain. Furthermore, the fire emissions in our set-up are represented using FINN v1, which uses the MODIS retrieved active fire locations to identify biomass burning regions. A recent study focused on sub-Saharan Africa suggested that the resolution of MODIS is too coarse to capture small scale fires and consequently MODIS burned area estimate can be lower by 80% compared to the burned area estimated with 20-m resolution of Sentinel-2 multispectral instrument (Ramo et al., 2021).

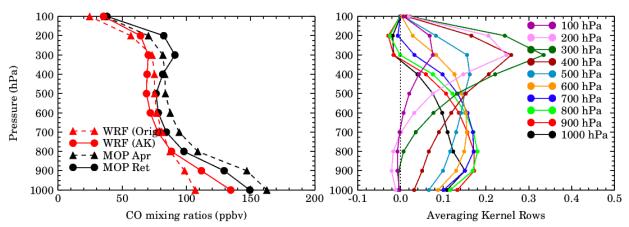


Figure 15: Comparison of the vertical distribution of MOPITT CO profiles against WRF-Chem CO profiles averaged over the CONUS during August 2019. WRF (orig) shows the raw vertical CO profile simulated by WRF-Chem and WRF (AK) shows the WRF-Chem CO vertical profile convolved with MOPITT a priori profile and averaging kernels. "MOP Apr" and "MOP Ret" represent the MOPITT a priori and retrieved profiles, respectively. Right panel: Vertical profiles of MOPITT averaging kernels corresponding to different pressure levels that are used in convolving the raw WRF-Chem CO profiles.

Comparisons are also conducted for selected time periods such as during large wildfire impacts. As an example, we show in Figure 16 a comparison of WRF-Chem AOD with MODIS derived AOD for 16 September 2020. The model fairly well represents the satellite derived AOD and the CO CONUS fire tracer, which is also shown and provides information on the CO attributed to fires within CONUS, suggests that the high aerosol concentrations are related to wildfires within CONUS.

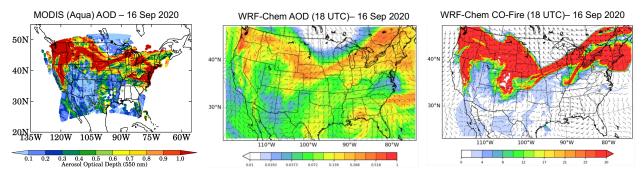


Figure 16: MODIS AOD (left), WRF-Chem AOD (middle) and CO CONUS fire tracer for 16 September 2020.

The assumption of linearity which allows the use of the tracer contribution in a linear way within the mitigation service was demonstrated in a previous study where we used CO tracers for the source attribution analysis of wintertime CO in India (Kumar et al., 2013). Figure 17 shows the spatial distribution of the percentage difference between total CO and sum of CO tracers (anthropogenic emissions, fire emissions, biogenic emissions, photochemical production, and inflow from the lateral domain boundaries) at the surface on 10, 20, and 31 Dec 2007 at 00 UTC.

The model simulations for this study started on 01 Dec 2007 at 00 UTC. At the surface, the percentage differences between the instantaneous total CO and the sum of CO tracers show that the sum of all tracers approaches total CO values after about 20 days (Figure 17) with values within 5% of total CO surface over the land region of South Asia. It is 10–15% over the Oceanic region (Arabian Sea). The tracers are well spun up at the surface after 31 days with percent difference of less than 2% over the domain and remaining within 2% throughout the simulation. In the free troposphere, all the tracers are found to spin up well after 10 days of the model run.

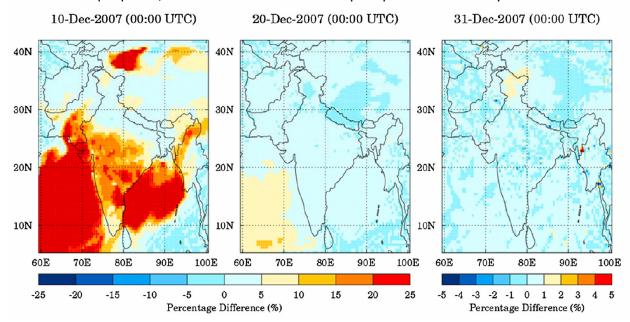


Figure 17: spatial distribution of the percentage difference between total CO and sum of CO tracers on 10, 20, and 31 Dec 2007 at 00 UTC. Note different color scales for different panels. Figure reproduced from Kumar et al., (2013)

4.5 Operational implementation of the AQ-WATCH AQ mitigation tool

The PM and CO mitigation service systems based on the LOTOS-EUROS and WRF-CHEM models are currently running operationally and being implemented in the AQ-WATCH toolkit.

Figure 18 shows the concept of the mitigation service interface, with sliders below the map, where the user can choose to reduce emissions from specific sources (more information in Sections 4.3, 4.5 and 4.4). The impact of these emission reductions on the pollutant concentrations in the region of interest is shown in the map. Below the map, the time variation of the pollutant of choice will be shown, for the past 6 weeks and 48h forecast, for any user-defined location in the domain, before and after the chosen emission reductions. Note that the figure does not show actual data from the models yet. Although the service is currently running operationally, the data from the operational data streams is in the process of being included in the AQ-WATCH toolkit.

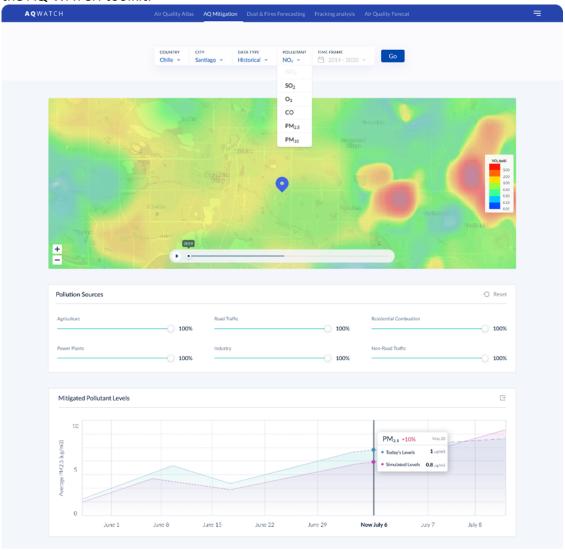


Figure 18: Mockup of mitigation service in the AQ-WATCH interface

4.6 Local PM, NO₂ and O₃ mitigation service with SIRANet

SIRANE model

SIRANE (Soulhac et al., 2011, http://air.ec-lyon.fr/SIRANE/index.php?Lang=EN) is an urban local scale dispersion model developed by the LMFA (Laboratory and Fluid transfer and Acoustic). It is widely used in France, Europe and beyond to perform air quality simulation at urban street level scale. The model is parallelized so that it can consider large number (up to tens of thousands) of roads sections. Below the urban canopy, the model consists of a network of connected street segments and parameterizations of transport processes between these segments. Above the urban canopy, it consists of a parameterization of the atmospheric boundary layer, coupled to a Gaussian model for the dispersion above the roof level.

Considering the effect of regional background air pollution on the air quality at the street level, a multi-scale (China-BTH-City-Street) air quality forecasting model suite from the regional to local scale with nested CHIMERE-SIRANE models is installed and works every day to provide up to 4 days forecast. The details of CHIMERE model used for Chinese region in AQ-WATCH are described in the Deliverable D3.1. In general, CHIMERE is launched to simulate the regional and city scale air quality. Taking outputs of city level simulation from CHIMERE as the inputs of boundary conditions, the SIRANE model is used to simulate the street level air quality. Figure 19 provides a schematic of the CHIMERE-SIRANE forecast system. The detailed set-up is described in the next sections.

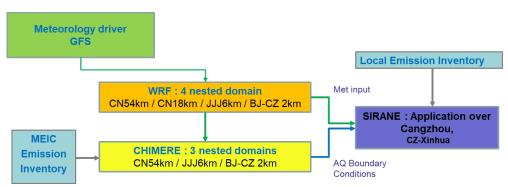


Figure 19: Architecture of the IUSE air quality forecasting system

Mitigation service method with SIRANet

SIRANE requires about 30 minutes to run a 5-day forecast which is too time consuming to perform many scenarios in an operational setting as required in the mitigation service.

To this end we developed a new model (which we will call "metamodel") based on the simplification of the atmospheric dispersion model SIRANE to perform fast simulations. the metamodel is based on Artificial Intelligence (AI) techniques and can run in 1 minute maximum thereby offering the possibility to deliver a quick response. The chain under development relies

on the capabilities of a UNet-based architecture involving Convolutional Neural Networks (CNN) to perform model emulation. To meet this objective, the neural network will need to be properly structured and trained. For general information, a neural network uses a training dataset to optimize the weights in its architecture. The set of trained parameters will then be used for application on new datasets. Once the training performance of the neural network is satisfactory, it can be used as many times as needed.

Hereby, a tool (here SIRANet) is developed based on a PyTorch Lightning implementation, to quickly analyze air pollution mitigation strategies at Xinhua district, Cangzhou domain. The basic concepts of SIRANet are illustrated in Figure 20. The SIRANE inputs are used to train a deep learning-based emulator, which can ease their use within the neural network. To facilitate their use within the neural network, these inputs are mapped on a grid with the same dimensions as the output 10 m × 10 m grid. Considering the spatial structure of the two-dimensional data set corresponding to the surface concentration field of pollutants, a PyTorch-based implementation is proposed to use UNet-based CNN to extract information (mainly emissions and weather data) from the inputs of the SIRANE model and present a fast high-resolution simulation. The AWS mono-GPU virtual machine is used to train a neural network. After the training step, these parameters are used for application on to any new dataset.

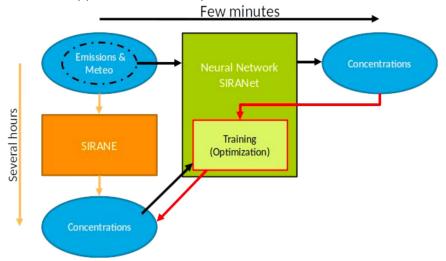


Figure 20: Basic concepts of SIRANet.

System set-up

So far, the nested CHIMERE-SIRANE models are installed and available on a CPU infrastructure and running operationally every day at the BCC institute to provide up to 4 days forecast. CHIMERE is launched on the 3 nested domains d01, d03 and d05 (see Figure 21), where d01 is the coarse China continental domain at 54km resolution, d03 is the regional domain including Beijing and Cangzhou city at 6 km resolution, and d05 is the local domain at Cangzhou city at 2 km resolution. The meteorology input for CHIMERE comes from the Weather Research and Forecast (WRF) model (Skamarock et al., 2008) results from domains d01 and d03 (the d02 WRF domain is merely an intermediary step in the WRF downscaling process).

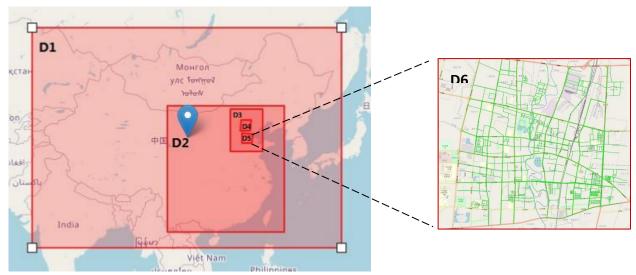


Figure 21: illustration of the domains used for WRF (d01, d02, d03), CHIMERE (d01, d03, d05) and SIRANE(d6). D4 is not used in this WP. The street network considered in the SIRANE model over Xinhua district, Cangzhou is showed in the right panel.

For the street level scale with SIRANE, the domain over a Cangzhou center district (Xinhua District) is at 10 meters resolution. The SIRANE local forecast considers the CHIMERE forecast output from Cangzhou domain as boundary conditions. First, an extraction of the required meteorological parameters is done from the WRF simulation. Once knowing the wind direction, the concentration used as boundary conditions is taken from the point upstream of the CHIMERE grid. In a second step, the simulations are launched on the domain.

In the SIRANet, the modelling domain is Xinhua district, Cangzhou city in China. The street network considered for the modelling is shown in Figure 21 (right panel). It includes the emission of 4651 road sections. Two emission sectors including road traffic and residential sectors are currently targeted. The industrial sector will be added later. Meanwhile, the target pollutants are PM, NO₂ and O₃. Once trained for all the pollutants, the models can be used in the operational workflow. The application of the model on new datasets simply takes three arguments: (1) the input SIRANE files (meteorological parameters, background mesoscale concentration, emissions) which are stored as a NetCDF file, (2) the prefix of the experiments (xp_large, xp_small, etc), and (3) the neural network scaling model (S1/S2). The inference is finally made by the high-resolution neural network outputs. The files are uploaded to the distant AWS GPU virtual machine, and the SIRANet predictions are run from start and end date given by the end-user. The output can be downloaded as a NetCDF file, with similar structure as SIRANE outputs. The operational service currently can produce 24 hourly predictions for each pollutant.

Results

A R-shiny-based user interface is established to allow the users to define the appropriate scenario based on the targeted emission sectors and will send on-the-fly the corresponding run on the computing system interactively. Three panels are integrated in a the R-shiny Dashboard page to ease the use of SIRANet from an end-user perspective (see Figure 22): Panel #1 (the top left of Figure 22): road + residential emission (in current stage, residential emission only included cooking emission) sliders to define the scenarios & a calendar for start and end date of the predictions; Panel #2 (the right of Figure 22): a Leaflet map to display the SIRANet outputs and Panel #3 (the bottom left of Figure 22): a time series to display some statistics based on the scenarios already ran by the end-user. Previous run scenario results are stored locally as NetCDF files on the local computer or on a server according to where the webapp is deployed.

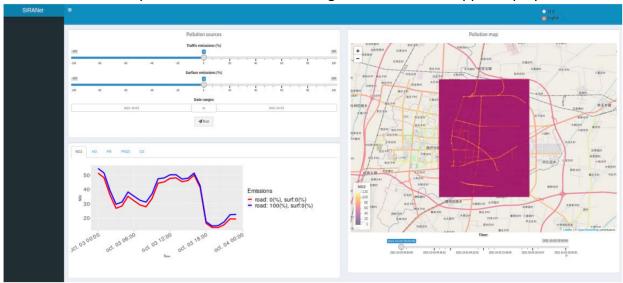


Figure 22: Shiny-based interface of SIRANet scenario assessment.

Evaluation

The performance of the neural network approach is evaluated according to three indicators: visualization capacity, model evaluation statistics and computational performance. The concentration maps produced by the network are realistic and similar to the ones produced by the SIRANE model (see example in Figure 23). The model may reproduce lower O_3 concentrations within the streets due to the titration effects. Meanwhile, the network predictions do meet expected performance levels on metrics such as correlation (>0.7 near the main traffic axes and >0.9 in the background) and root mean square deviation (RMSE <10 $\mu g/m^3$ near the main traffic axes and <5 $\mu g/m^3$ in the background) indicating generally very satisfactory performances. Future improvements will be made by focusing network training near major emissions areas and industrial point sources.

The operational service currently produces 24-hour predictions for a pollutant in less than a minute (data loading included). This should be considerably improved according to the GPU configuration used for the operational setup.

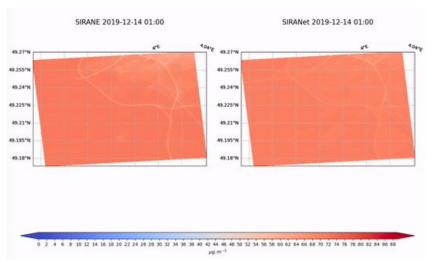


Figure 23: example of SIRANet performance (O_3) . Left panel is the simulated concentration from SIRANE, and right panel is the simulated concentration from SIRANet.

Operational implementation

The SIRANet is running operational and can be used through an R-shiny- based interface. This interface can be used on a local server after the installation of the user interface execution package. The operational service currently produces 24-hour predictions for a pollutant in less than a minute (data loading included). This should be considerably improved according to the GPU configuration used for the operational setup. Due to the data policy in China, SIRANet will run as an independent tool and will not be incorporated as part of the AQ-WATCH AQ Mitigation Tool. However, the SIRANet interface will be linked to the AQ-WATCH AQ mitigation module upon the completion of the service development.

4.7 Next steps and recommendations

PM mitigation service with LOTOS-EUROS: The operational service will be made available through the AQ-WATCH interface. In the evaluation of the source attribution service, it was found that the model underestimates observed NO₂ and PM concentrations, when using CAMS-global emissions (see deliverable report 4.1 on the source attribution service). Therefore, we recommend implementing local high resolution emission inventories, and in regions with large orographic variations also high-resolution meteorology to reach better model performance before utilizing results from the attribution and mitigation service. Further, before applying the developed mitigation service over any new region, a new evaluation on the set-up of the service and the chosen 12 runs on which the surrogate model is based should take place. Because we consider also interactions between different sources, an extension of the service to additional sectors would require additional model runs and considerable complication of the equation underlying the current service. Since we found that the emission-concentration relationship for

power plants acts mostly linear, it would be possible to include this sector under the assumption of linear response. For further extension to additional sectors, exploring other methods might be worthwhile.

CO mitigation service with WRF-Chem: The operational service will be made available through the AQ-WATCH toolkit. As a part of WP 6, the service will be demonstrated to the prime users in Colorado and adjustments to the CO tracers (e.g. addition of new tracers, modification to existing sources/regions) will be made following their feedback. In addition, UCAR will continue evaluation of the forecasts and also assess whether the quality of current operational CO surface monitoring data is sufficient for evaluating the model.

Mitigation service China: More work will be done to improve the performance of the street scale simulations especially for heavy pollution days, the neural network architecture to embed efficient dispersion processes schemes, and to speed up the inference with multi-GPU implementation. Besides, the implementation of the whole software (shiny interface + SIRANet python toolbox) on the same server needs to be solved to ease the communication and transfer speed-related issues.

5. References (Bibliography)

- Banzhaf, S., Schaap, M., Kerschbaumer, A., Reimer, E., Stern, R., Van Der Swaluw, E., Builtjes, P., 2012. Implementation and evaluation of pH-dependent cloud chemistry and wetdeposition in the chemical transport model REM-Calgrid. Atmos. Environ. 49. https://doi.org/10.1016/j.atmosenv.2011.10.069
- Chin, M., Rood, R.B., Lin, S.J., Müller, J.F., Thompson, A.M., 2000. Atmospheric sulfur cycle simulated in the global model GOCART: Model description and global properties. J. Geophys. Res. Atmos. 105, 24671–24687. https://doi.org/10.1029/2000JD900384
- Colette, A., Rouïl, L., Meleux, F., Lemaire, V., Raux, B., 2022. Air Control Toolbox (ACT_v1.0): A flexible surrogate model to explore mitigation scenarios in air quality forecasts. Geosci. Model Dev. 15, 1441–1465. https://doi.org/10.5194/GMD-15-1441-2022
- Crippa, M., Guizzardi, D., Muntean, M., Schaaf, E., Dentener, F., Van Aardenne, J.A., Monni, S., Doering, U., Olivier, J.G.J., Pagliari, V., Janssens-Maenhout, G., 2018. Gridded emissions of air pollutants for the period 1970-2012 within EDGAR v4.3.2. Earth Syst. Sci. Data 10, 1987–2013. https://doi.org/10.5194/ESSD-10-1987-2018
- Emmons, L.K., Schwantes, R.H., Orlando, J.J., Tyndall, G., Kinnison, D., Lamarque, J.F., Marsh, D., Mills, M.J., Tilmes, S., Bardeen, C., Buchholz, R.R., Conley, A., Gettelman, A., Garcia, R., Simpson, I., Blake, D.R., Meinardi, S., Pétron, G., 2020. The Chemistry Mechanism in the Community Earth System Model Version 2 (CESM2). J. Adv. Model. Earth Syst. 12, e2019MS001882. https://doi.org/10.1029/2019MS001882
- Flemming, J., Huijnen, V., Arteta, J., Bechtold, P., Beljaars, A., Blechschmidt, A.M., Diamantakis, M., Engelen, R.J., Gaudel, A., Inness, A., Jones, L., Josse, B., Katragkou, E., Marecal, V., Peuch, V.H., Richter, A., Schultz, M.G., Stein, O., Tsikerdekis, A., 2015. Tropospheric chemistry in the integrated forecasting system of ECMWF. Geosci. Model Dev. 8, 975–1003. https://doi.org/10.5194/GMD-8-975-2015
- Fountoukis, C., Nenes, A., 2007. ISORROPIAII: A computationally efficient thermodynamic equilibrium model for K+-Ca2+-Mg2+-NH4 +-Na+-SO42--NO3 --Cl--H2O aerosols. Atmos. Chem. Phys. 7, 4639–4659.
- Freitas, S.R., Longo, K.M., Chatfield, R., Latham, D., Silva Dias, M.A.F., Andreae, M.O., Prins, E., Santos, J.C., Gielow, R., Carvalho, J.A., 2007. Including the sub-grid scale plume rise of vegetation fires in low resolution atmospheric transport models. Atmos. Chem. Phys. 7, 3385–3398. https://doi.org/10.5194/ACP-7-3385-2007
- Gery, M.W., Whitten, G.Z., Killus, J.P., Dodge, M.C., 1989. A photochemical kinetics mechanism for urban and regional scale computer modeling. J. Geophys. Res. Atmos. 94, 12925–12956. https://doi.org/10.1029/JD094ID10P12925
- Ginoux, P., Chin, M., Tegen, I., Prospero, J.M., Holben, B., Dubovik, O., Lin, S.J., 2001. Sources and distributions of dust aerosols simulated with the GOCART model. J. Geophys. Res. Atmos. 106, 20255–20273. https://doi.org/10.1029/2000JD000053
- Granier, C., S. Darras, H. Denier van der Gon, J. Doubalova, N. Elguindi, B. Galle, M. Gauss, M. Guevara, J.-P. Jalkanen, J. Kuenen, C. Liousse, B. Quack, D. Simpson, K. Sindelarova, 2019. The Copernicus Atmosphere Monitoring Service global and regional emissions (April 2019 version). https://doi.org/10.24380/d0bn-kx16
- Grell, G.A., Peckham, S.E., Schmitz, R., McKeen, S.A., Frost, G., Skamarock, W.C., Eder, B., 2005.

- Fully coupled "online" chemistry within the WRF model. Atmos. Environ. 39, 6957–6975. https://doi.org/10.1016/J.ATMOSENV.2005.04.027
- Guenther, A.B., Jiang, X., Heald, C.L., Sakulyanontvittaya, T., Duhl, T., Emmons, L.K., Wang, X., 2012. The model of emissions of gases and aerosols from nature version 2.1 (MEGAN2.1): An extended and updated framework for modeling biogenic emissions. Geosci. Model Dev. 5, 1471–1492. https://doi.org/10.5194/GMD-5-1471-2012
- Hoesly, R.M., Smith, S.J., Feng, L., Klimont, Z., Janssens-Maenhout, G., Pitkanen, T., Seibert, J.J., Vu, L., Andres, R.J., Bolt, R.M., Bond, T.C., Dawidowski, L., Kholod, N., Kurokawa, J.I., Li, M., Liu, L., Lu, Z., Moura, M.C.P., O'Rourke, P.R., Zhang, Q., 2018. Historical (1750-2014) anthropogenic emissions of reactive gases and aerosols from the Community Emissions Data System (CEDS). Geosci. Model Dev. 11, 369–408. https://doi.org/10.5194/GMD-11-369-2018
- Kaiser, J.W., Heil, A., Andreae, M.O., Benedetti, A., Chubarova, N., Jones, L., Morcrette, J.-J., Razinger, M., Schultz, M.G., Suttie, M., van der Werf, G.R., 2012. Biomass burning emissions estimated with a global fire assimilation system based on observed fire radiative power. Biogeosciences 9, 527–554. https://doi.org/10.5194/bg-9-527-2012
- Kumar, R., Bhardwaj, P., Pfister, G., Drews, C., Honomichl, S., D'attilo, G., 2021. Description and Evaluation of the Fine Particulate Matter Forecasts in the NCAR Regional Air Quality Forecasting System. Atmos. 2021, Vol. 12, Page 302 12, 302. https://doi.org/10.3390/ATMOS12030302
- Kumar, R., Naja, M., Pfister, G.G., Barth, M.C., Brasseur, G.P., 2013. Source attribution of carbon monoxide in India and surrounding regions during wintertime. J. Geophys. Res. Atmos. 118, 1981–1995. https://doi.org/10.1002/JGRD.50134
- Manders, A.M.M., Builtjes, P.J.H., Curier, L., Denier van der Gon, H.A.C., Hendriks, C., Jonkers, S., Kranenburg, R., Kuenen, J., Segers, A.J., Timmermans, R.M.A., Visschedijk, A., Wichink Kruit, R.J., Van Pul, W.A.J., Sauter, F.J., van der Swaluw, E., Swart, D.P.J., Douros, J., Eskes, H., van Meijgaard, E., van Ulft, B., van Velthoven, P., Banzhaf, S., Mues, A., Stern, R., Fu, G., Lu, S., Heemink, A., van Velzen, N., Schaap, M., 2017. Curriculum Vitae of the LOTOS-EUROS (v2.0) chemistry transport model. Geosci. Model Dev. 10, 4145–4173. https://doi.org/10.5194/gmd-10-4145-2017
- Marsh, D.R., Mills, M.J., Kinnison, D.E., Lamarque, J.F., Calvo, N., Polvani, L.M., 2013. Climate Change from 1850 to 2005 Simulated in CESM1(WACCM). J. Clim. 26, 7372–7391. https://doi.org/10.1175/JCLI-D-12-00558.1
- Neu, J.L., Prather, M.J., 2012. Toward a more physical representation of precipitation scavenging in global chemistry models: Cloud overlap and ice physics and their impact on tropospheric ozone. Atmos. Chem. Phys. 12, 3289–3310. https://doi.org/10.5194/ACP-12-3289-2012
- Powers, J.G., Klemp, J.B., Skamarock, W.C., Davis, C.A., Dudhia, J., Gill, D.O., Coen, J.L., Gochis, D.J., Ahmadov, R., Peckham, S.E., Grell, G.A., Michalakes, J., Trahan, S., Benjamin, S.G., Alexander, C.R., Dimego, G.J., Wang, W., Schwartz, C.S., Romine, G.S., Liu, Z., Snyder, C., Chen, F., Barlage, M.J., Yu, W., Duda, M.G., 2017. The Weather Research and Forecasting Model: Overview, System Efforts, and Future Directions. Bull. Am. Meteorol. Soc. 98, 1717–1737. https://doi.org/10.1175/BAMS-D-15-00308.1

- Ramo, R., Roteta, E., Bistinas, I., van Wees, D., Bastarrika, A., Chuvieco, E., van der Werf, G.R., 2021. African burned area and fire carbon emissions are strongly impacted by small fires undetected by coarse resolution satellite data. Proc. Natl. Acad. Sci. 118. https://doi.org/10.1073/PNAS.2011160118
- Skamarock, W.C., Klemp, J.B., Dudhia, J., Gill, D.O., Barker, D.M., Duda, M.G., Huang, X.-Y., Wang, W., Powers, J.G., 2008. A Description of the Advanced Research WRF Version 3. https://doi.org/10.5065/D68S4MVH
- Soulhac, L., Salizzoni, P., Cierco, F.X., Perkins, R., 2011. The model SIRANE for atmospheric urban pollutant dispersion; part I, presentation of the model. Atmos. Environ. 45, 7379–7395. https://doi.org/10.1016/J.ATMOSENV.2011.07.008
- Van Zanten, M.C., Sauter, F.J., Wichink Kruit, R.J., Van Jaarsveld, J.A., Van Pul, W.A.J., 2010. Description of the DEPAC module: Dry deposition modelling with DEPAC GCN2010. RIVM Rep. 680180001/2010.
- Wang, K., Gao, J., Liu, K., Tong, Y., Dan, M., Zhang, X., Liu, C., 2022. Unit-based emissions and environmental impacts of industrial condensable particulate matter in China in 2020. Chemosphere 303, 134759. https://doi.org/10.1016/J.CHEMOSPHERE.2022.134759
- Wesely, M.L., 1989. Parameterization of surface resistances to gaseous dry deposition in regional-scale numerical models. Atmos. Environ. 23, 1293–1304. https://doi.org/10.1016/0004-6981(89)90153-4
- Wichink Kruit, R.J., Schaap, M., Sauter, F.J., Swaluw van der, E., Weijers, E., 2012. Improving the understanding of the secondary inorganic aerosol distribution over the Netherlands, TNO-report TNO-060-UT-2012-00334.
- Wichink Kruit, R. J., Schaap, M., Sauter, F.J., van Zanten, M.C., van Pul, W.A.J., 2012. Modeling the distribution of ammonia across Europe including bi-directional surface—atmosphere exchange. Biogeosciences 9, 5261–5277. https://doi.org/10.5194/bg-9-5261-2012
- Wiedinmyer, C., Akagi, S.K., Yokelson, R.J., Emmons, L.K., Al-Saadi, J.A., Orlando, J.J., Soja, A.J., 2011. The Fire INventory from NCAR (FINN): A high resolution global model to estimate the emissions from open burning. Geosci. Model Dev. 4, 625–641. https://doi.org/10.5194/GMD-4-625-2011
- Zhang, L., 2001. A size-segregated particle dry deposition scheme for an atmospheric aerosol module. Atmos. Environ. 35, 549–560. https://doi.org/10.1016/S1352-2310(00)00326-5

6. Dissemination and uptake

6.1 Uptake by the targeted audience

As indicated in the Description of the Action, the audience for this deliverable is

X	The general public (PU)
	The project partners, including the Commission services (PP)
	A group specified by the consortium, including the Commission services (RE)
	This report is confidential, only for members of the consortium, including the Commission
	services (CO)

6.2 This is how we are going to ensure the uptake of the deliverables by the targeted audience

- The latest version of the service will be presented to the prime users in Colorado and Chile in 2022.
- The service will also be presented at several public events (e.g. the air quality conference, LOTOS-EUROS workshops)
- The deliverable will be circulated within the consortium via the link: https://owncloud.gwdg.de/index.php/s/EQWP438kM2xhGNb

7. Deliverable timeliness

Is the deliverable delayed?

Yes □ No

Justification: The development of the source attribution tool interface was delayed. Additional time was necessary to obtain the screenshots of the latest version of the interface for the completeness of this deliverable.

8. Changes made and/or difficulties encountered, if any

Not applicable

9. Sustainability

9.1 Lessons learnt: both positive and negative that can be drawn from the experiences of the work to date

Not applicable

9.2 Links built with other deliverables, WPs, and synergies created with other projects

The mitigation service is based on air quality forecasts developed within WP3, partly on the source attribution service developed in WP4, and the description of the AQ-WATCH Toolkit interface in WP5. This deliverable is therefore linked to Deliverable 3.1, 4.1 and 5.5.

10. Full track of dissemination activities

Type of dissemination and communication activities	Details	Location , dates	Audience	Link in website (if applicable)	Estimated number of persons reached
Participation	Renske	27 June - 1	Scientific	https://www.	50 - 100
to a	Timmermans	July 2022,	Community	herts.ac.uk/ai	
conference	(TNO), AQ-	Hybrid form:	(higher	<u>rqualityconfe</u>	
	WATCH'S AIR	Thessaloniki	education,	<u>rence</u>	
	QUALITY	(GR) and	Research)		
	SOURCE	online	Industry		
	ATTRIBUTIO		Policy		
	N AND		makers		
	MITIGATION		Customers		
	SERVICE, AQ				
	Conference				

11. Full track of publications and IP

11.1 Peer reviewed articles

Not applicable

11.2 Publications in preparation OR submitted:

Not applicable

11.3 Intellectual property rights resulting from this deliverable:

The mitigation tool based on LOTOS-EUROS which was developed in AQ-WATCH, was a result of the work of a single partner (TNO). Following the grant agreement, TNO will therefore be the exclusive owner of this tool.