HTAP3-OPNS: Ozone, PM, Nitrogen and Sulphur Deposition - multi-model experiments to support the revision of the CLRTAP Gothenburg Protocol

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Abstract. HTAP3-OPNS is a multi-model exercise designed to support the revision of the Gothenburg Protocol under the UNECE Convention on Long-Range Transboundary Air Pollution (CLRTAP). Using an ensemble of Chemical Transport Models (CTMs) and Chemistry-Climate Models (CCMs), this study investigates the long-range transport and impacts of ground-level ozone, particulate matter (PM), and nitrogen and sulphur deposition across different global regions. The project aims to assess the contributions of regional versus extra-regional emission sources, evaluate the suitability of current models, and project changes in air pollution under future emission scenarios and climate conditions. A series of perturbation simulations will enable the development of an ensemble emulator to explore and evaluate various mitigation strategies efficiently. This paper outlines the scientific and policy questions motivating the study, describes the experimental design, including input datasets, model configurations, and required outputs, and discusses methodologies for data handling and analysis. The results will provide crucial insights for policy decisions aiming to improve air quality, protect human health, and protect ecosystems worldwide.

1 Introduction

The 1999 Gothenburg Protocol (GP) of the United Nations Economic Commission for Europe (UNECE) Convention on Long-Range Transboundary Air Pollution (CLRTAP) was the first international, multi-pollutant, multi-effect agreement aimed at reducing the negative effects of acidification, eutrophication, and ground-level ozone in Europe and North America. Under the GP, national emission reduction commitments were agreed for sulphur dioxide, nitrogen oxides, volatile organic compounds (VOCs) and ammonia, based on cost-effectiveness considerations. In 2012, the GP was amended to include particulate matter and black carbon, broadening its scope to include human health impacts and climate change co-benefits. A recent review of the GP concluded that current air quality legislation in the UNECE region is insufficient to meet CLRTAP's long-term clean air objectives. Furthermore, the review concluded that global reductions in methane emissions would be necessary to achieve these objectives.. The Executive Body (EB) of CLRTAP decided in its December 2023 session to launch the process of revising the GP and requested that the convention bodies contributing to the revisions specifically consider how methane in its role as an ozone precursor could be included in a future version of the GP.

The Task Force on Hemispheric Transport of Air Pollution (TF HTAP) was organized under the CLRTAP with the mandate to quantify the long-range (hemispheric to global) influence of distant sources of air pollution (including methane) in the UNECE region. Previous HTAP assessments (HTAP1 (HTAP, 2010) and HTAP2, https://acp.copernicus.org/articles/special_issue390.html) have shown that ground-level ozone is significantly influenced by long-range transport at the intercontinental scale and demonstrated the utility of a large ensemble of models for quantifying these effects and their uncertainty. While the primary policy audience of HTAP assessments is CLRTAP and UNECE member states, the work being organised here is also of scientific and policy significance for other world regions. To support the revisions of the GP, TF HTAP is currently organising a new round of multi-model experiments (HTAP3-OPNS) with the goal of quantifying the long-range contribution to ozone, particulate matter (PM), and the deposition of nitrogen (N) and sulfur (S) in different world regions.

In this document we describe the motivating science and policy questions, the design of the several different sets of experiments to be conducted to answer these questions, the input datasets to be used in carrying out these experiments, and the requested output data fields necessary for the analysis of the experiments and the answering of the science-policy questions.

2 Science-policy questions

The design of the HTAP3-OPNS multi-model experiments can be summarised by the following overarching questions.

- What are the contributions of intra-regional and extra-regional sources to air pollution and its impacts in different world regions?
- How suitable are current models for quantifying these contributions?
- Can we explain the inter-model differences?
- How will these contributions change under different realistic future emission scenarios and under potential future climate change?

While these overarching questions have also motivated previous HTAP assessments, there are several new aspects in HTAP3-OPNS.

- A stronger focus on the **impacts** of ground-level ozone, especially concerning damage to vegetation.
- A stronger focus on the effects of **methane** on ground-level ozone.
- A stronger focus on the effects of **wildfires** on long-range air pollution.
- A stronger focus on **total atmospheric deposition**, in support of the World Meteorological Organization (WMO) MMF-GTAD (Measurement-Model Fusion for Global Total Atmospheric Deposition) exercise. MMF-GTAD is organised by the WMO and aims to provide comprehensive maps of total atmospheric deposition through the fusion of all available deposition measurements with an ensemble of model runs.
- The use of **free-running future simulations** with atmospheric chemistry-climate models in addition to an ensemble emulator based on source-receptor relationships.
- Calculation of source/receptor relationships for air pollution based on a **future emissions scenario** rather than historical emissions.
- Comparison of **different methods for calculating source-receptor relationships**, such as source perturbation, tagging and adjoint techniques.

We also note that HTAP is currently involved in the organisation of two additional multi-model exercises, which are being coordinated with the HTAP3-OPNS exercise:

- **MCHgMAP** (Dastoor et al., 2024), organised together with the OESG (Open-Ended Science Group) of the Minamata Convention, with a focus on mercury and the first effectiveness evaluation of the Minamata Convention.
- **HTAP3-Fires** (Whaley et al., 2024), organised in cooperation with International Global Atmospheric Chemistry (IGAC) BBurned, with a focus on the impacts of wildfires on multiple pollutants (ozone, PM, Hg, POPs).

3 Future emission scenarios for the revision of the Gothenburg Protocol

The basis for all assessment of future air quality in HTAP3-OPNS will be the Greenhouse Gas - Air Pollution Interactions and Synergies (GAINS) LRTAP future emission scenarios, a set of emission scenarios produced using the GAINS model (Amann et al., 2011) of the International Institute for Applied Systems Analysis (IIASA), which serves as the EMEP Centre for Integrated Assessment Modelling (CIAM) under CLRTAP. Version 2.1 of the GAINS LRTAP scenarios was produced specifically to support the revision of the GP and is available for download (Klimont et al., 2025).

Model assessments in HTAP3-OPNS will use the “CLE” and “MTFR” scenarios from GAINS, as well as a hybrid “HILO” scenario, which are described in more detail below.

- CLE “Current Legislation”: This scenario is based on economic activity data broadly consistent with SSP2-4.5 (Riahi et al., 2017) and includes all current and planned air pollution control measures and their implementation timelines globally.

- MTFR “Maximum Technical Feasible Reduction”: This scenario is based on the same activity data as CLE but includes full implementation of all air pollution reduction measures (including methane reduction measures) which have been shown to be technically feasible (regardless of their cost effectiveness). Economic activity and associated CO_2 emissions are still broadly consistent with SSP2-4.5.
- HILO: In addition to the CLE and MTFR scenarios from GAINS, we construct an additional scenario for the purposes of HTAP3-OPNS combining the air pollutant emissions from MTFR and methane emissions from the CLE scenario. This hybrid scenario represents a policy pathway with high ambition on air pollution control, but with minimal ambition on methane control. Economic activity and associated CO_2 emissions are still broadly consistent with SSP2-4.5, as for both CLE and MTFR.

4 Overview of the requested model experiments

The model runs in HTAP3-OPNS are organised into three separate sets of experiments designed to answer the questions outlined above.

- **Perturbation experiments** with chemical transport models (CTMs) based on the GAINS LRTAP scenarios for the target year 2040.
- **Transient Future Scenario experiments** with chemistry climate models (CCMs) using the GAINS LRTAP scenarios from 2010 to 2050.
- **Transient Historical experiments** from 2003 to 2020 using a historical global mosaic emission inventory.

Modelling groups are requested to choose the sets of experiments to which they wish to contribute based on their capabilities, resources, and scientific interests.

4.1 Perturbation experiments for source-receptor relationships and ensemble emulation

As in previous HTAP assessments, we invite groups using global CTMs and CCMs (with specified dynamics from a reference meteorological base year) to perform source perturbation runs for key species/regions/sectors to allow the construction of source-receptor relationships. A key difference with previous HTAP assessments is that the proposed perturbation runs are based on emissions from a future scenario (CLE 2040 from the GAINS LRTAP scenarios) rather than from a historical reference year. The year 2040 is chosen to be consistent with the target year for air quality under the revision of the Gothenburg Protocol. The use of future emissions for the perturbation runs will enable direct construction of source-receptor relationships based on the future distribution of emissions. The key perturbation runs (species/regions/sectors) target the major Northern Hemisphere anthropogenic emission sources, and the model experiments in this set are described in more detail in Section 7.1. The development of the ensemble emulator is described in more detail in Section 8.2.2.

In addition to the standard base case and perturbation experiments based on CLE 2040 emissions, this set of experiments includes global model simulations of CLE 2015, MTFR 2040, and HILO 2040 using the same meteorological base year as the standard base case (CLE 2040). This set of four global CTM simulations (CLE 2015, CLE 2040, MTFR 2040, and HILO 2040) will provide boundary conditions for a set of regional model simulations using the GAINS LRTAP scenarios.

We also invite groups using alternative source attribution techniques such as tagging (e.g. Butler et al., 2020; Mertens et al., 2020) and adjoint sensitivity (e.g. Choi et al., 2019) to perform equivalent runs with their alternative methods and to contribute to the analysis of the different source attribution methods.

4.2 Transient future scenario experiments

In HTAP3-OPNS we invite modelling groups using atmospheric CCMs to contribute transient simulations for the period 2010-2050 using the GAINS LRTAP future anthropogenic emission scenarios and future fire emissions (Section 5.2). These simulations serve several purposes:

- Provide a direct assessment of the GAINS LRTAP scenarios.
- Act as a check on the output of the ensemble emulator produced from the Perturbation experiments.
- Allow quantification of the effects of climate change on long-range transport of air pollution.

A minimum of three simulations are requested in total from each modelling group (see Section 7.4 for more details).

4.3 Transient historical experiment

We invite groups using CTMs and CCMs to perform specified dynamics simulations from 2003-2020 using standardised historical emission inventories for anthropogenic emissions and biomass burning. These simulations serve several purposes:

- Provide an assessment of the models' ability to simulate observed trends and interannual variability.
- Comprehensive deposition fields from these runs will be provided to the WMO for use in the MMF-GTAD project (https://community.wmo.int/en/activity-areas/gaw/science-for-services/mmf-gtad).
- Provide a baseline simulation for additional experiments in the related HTAP3-Fires exercise (Whaley et al., 2024).

The Transient Historical experiment is described in more detail in Section 7.5.

4.4 Global to regional downscaling

Regional modelling groups are invited to perform simulations for their region of interest using the GAINS LRTAP emission scenarios and boundary conditions from the global CTMs contributing to HTAP3-OPNS through the Perturbation experiments (Section 4.1).

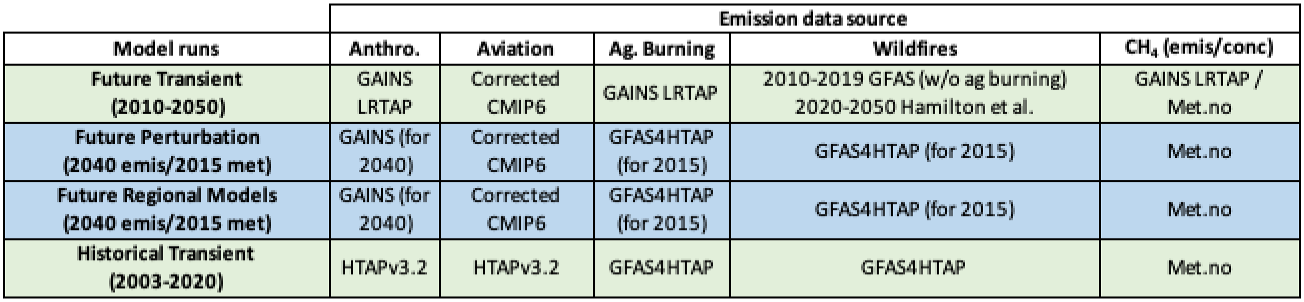
For the European domain, TF HTAP will organise a common set of model experiments designed to support the revision of the GP in cooperation with the CLRTAP Task Force on Measurements and Modelling (TFMM) and the Copernicus Atmosphere Monitoring Service (CAMS). These experiments are described in more detail in Section 7.3.

4.5 Additional science questions

Some groups may see an opportunity to piggyback on the HTAP3-OPNS multi-model exercise to answer additional scientific questions (e.g., detailed analysis of ozone budgets, deposition pathways, regionally focused assessments, etc…) and to take a leadership role in the associated analysis. These groups are encouraged to discuss their ideas at TF HTAP meetings and potentially recruit other modelling groups to participate by contributing additional runs or model output parameters.

5 Input data sets

All HTAP3-OPNS model experiments will require modelling groups to use standardised emission datasets for anthropogenic and biomass burning emissions for the defined simulation periods. All other aspects of model configuration, such as natural emissions and meteorological forcing will be left to the discretion of each modelling group, as long as these are consistent with the overall climate forcing required for each model run, which is described for each set of experiments below.



	Emission data source				
Model runs	**Anthro.**	**Aviation**	**Ag. Burning**	**Wildfires**	**CH_4 (emis/conc)**
Future Transient (2010-2050)	GAINS LRTAP	Corrected CMIP6	GAINS LRTAP	2010-2019 GFAS (w/o ag burning) 2020-2050 Hamilton et al.	GAINS LRTAP / Met.no
Future Perturbation (2040 emis/2015 met)	GAINS (for 2040)	Corrected CMIP6	GFAS4HTAP (for 2015)	GFAS4HTAP (for 2015)	Met.no
Future Regional Models (2040 emis/2015 met)	GAINS (for 2040)	Corrected CMIP6	GFAS4HTAP (for 2015)	GFAS4HTAP (for 2015)	Met.no
Historical Transient (2003-2020)	HTAPv3.2	HTAPv3.2	GFAS4HTAP	GFAS4HTAP	Met.no

Table 1 Summary of the emission datasets to be used in each of the experiment sets in HTAP3-OPNS

Table 1 shows the emission datasets which should be used for each of the different experiment sets in HTAP3-OPNS. The individual datasets are described in more detail below.

5.1 Anthropogenic future emission scenarios

All model experiments in the Perturbation and Transient Future Scenario sets of experiments must use the GAINS LRTAP version 2.1 anthropogenic emission scenarios. This dataset was introduced in Section 3.

The GAINS LRTAP version 2.1 emissions for the CLE and MTFR scenarios are available for download from (Klimont et al., 2025) and contain the following emission sectors:

- Energy sector
- Residential combustion (cooking and heating)
- Transportation
- Industry (combustion and processes)
- Solvent use
- Waste management
- Agriculture (livestock and fertilizer application)
- Open burning of agricultural residues
- International shipping

The hybrid HILO scenario is not included in the official GAINS set of scenarios, but must rather be constructed by each modelling group by taking methane emissions from the CLE scenario and emissions of all other pollutants from the MTFR scenario. For CTMs and other models using prescribed methane concentrations, methane concentrations are available for all three scenarios (CLE, MTFR, and HILO, see Section 5.5).

The GAINS LRTAP scenarios do not provide emissions for the aviation sector. All sets of experiments in HTAP3-OPNS which use GAINS LRTAP scenarios (the Perturbation and Transient Future Scenarios experiments) should use aircraft emissions from the CMIP6 historical and SSP2-4.5 datasets as appropriate for the simulation period. The vertical distribution should be kept as provided in the emission files (with appropriate interpolation to the vertical levels of each participating model to be performed by each group themselves). The correction described in Thor et al. (2023) should be applied to the CMIP6 aircraft emissions. Corrected CMIP6 historical emissions for aviation are available for download from (Mertens, 2024a). Corrected SSP2-4.5 scenario emissions for aviation are available for download from (Mertens et al., 2024b).

The GAINS LRTAP sector “Open burning of agricultural residues” should be excluded from the Perturbation experiments, which use the historical biomass burning emissions from GFAS4HTAP (Section 5.3), as the GFAS4HTAP emissions already include this source. Conversely, the GAINS LRTAP agricultural burning emissions should be included in the Transient Future Scenarios experiments, as the future fire emissions for this set of experiments do not include managed burning. Table 1 provides a summary of the emissions to be used in each set of experiments.

Modelling groups are free to choose their own chemical speciation profiles, temporal profiles, and injection heights for the GAINS LRTAP scenarios.

5.2 Future fire emissions

All model experiments in the Transient Future Scenario set of experiments (Section 4.2) must use the dataset from Bergas-Massó and Hamilton (2025). Future biomass burning emissions from wildfires in this dataset have been prepared based on the output from an ensemble of ESMs with interactive fire models, bias corrected to present-day GFAS4HTAP emissions (Section 5.3). These future fire emission datasets correspond to climates simulated in SSP2-4.5 and will also be considered for use in other related multi-model exercises coordinated through HTAP3-Fires, IGAC-BBURNED, and AMAP.

For the model spinup and the period 2010-2019, modelling groups should use biomass burning emissions from GFAS4HTAP (Section 5.3). From 2020 onwards, the Bergas-Massó and Hamilton (2025) emissions should be used.

The Bergas-Massó and Hamilton (2025) dataset does not include burning of agricultural waste. As shown in Table 1, all model experiments in the Transient Future Scenario set of experiments should take emissions from agricultural waste burning from the GAINS LRTAP scenarios (Section 5.1).

Recommended injection heights for future fires follow (Dentener et al., 2006).

5.3 Historical fire emissions

As shown in Table 1, all model experiments performed in the Perturbation and Transient Historical sets of experiments must use all sectors including agricultural waste burning) from the GFAS4HTAP dataset (Kaiser et al., 2023) which has been developed specifically for HTAP3-OPNS and HTAP3-Fires. To ensure maximum overlap between these related exercises, a common biomass burning emission dataset will be used in both HTAP3-OPNS and HTAP3-Fires.

5.4 Historical anthropogenic emissions

All model experiments in the Transient Historical set of experiments must be based on the monthly mean fluxes for 2000-2020 from HTAPv3.2 (Guizzardi et al., 2025), an update to the HTAPv3 global mosaic emission inventory (Crippa et al., 2023). The HTAPv3.2 dataset is available for download from Zenodo (Crippa, 2024).

Agricultural waste burning emissions from HTAPv3.2 should be excluded from the Transient Historical experiments (Table 1), since these are included in the biomass burning emissions from GFAS4HTAP (Section 5.3). Modelling groups are encouraged to use the NMVOC speciation profiles provided with the HTAPv3.2 emission inventory. Modelling groups are free to apply vertical emission profiles to these emissions as they see fit, although HTAP makes no specific recommendation on vertical emission profiles.

The Historical Transient experiment is the only experiment in HTAP3-OPNS using the HTAPv3.2 emission inventory (Table 1). For the historical component of the Transient Future and Perturbation sets of experiments, emissions are taken from the GAINS LRTAP scenarios (Section 5.1).

5.5 Surface methane emissions and concentrations

For the Transient Future set of experiments, anthropogenic emissions of methane are provided in the GAINS LRTAP future scenarios (Section 5.1). Groups with the capacity to perform methane emission-driven simulations should use the GAINS LRTAP anthropogenic methane emission fluxes, along with their own choice of natural methane emissions and any necessary flux adjustment (Folberth et al., 2022).

For all groups performing the Perturbation experiments, and for groups performing the Transient Future experiments without the capacity to perform methane emission-driven simulations, surface concentrations of methane consistent with the GAINS LRTAP emission scenarios CLE and MTFR and the hybrid scenario HILO are provided based on the reduced complexity climate model (RCM) simulations run by MSC-W (Met Norway) driven by emissions from the GAINS LRTAP scenarios. In HTAP3-OPNS, these methane concentrations are named as Met.no. The RCM used for this purpose is the Model for the Assessment of Greenhouse-gas Induced Climate Change v7.5.3, MAGICC7 (Meinshausen et al., 2009, 2011, 2020), following the approach described in Van Caspel et al. (2024). In this configuration, the MAGICC7 model is run in its 600-ensemble probabilistic mode (Nicholls et al., 2021) to calculate global mean tropospheric methane concentrations as a function of the anthropogenic emission scenarios. Natural emissions are estimated by closing the methane budget with respect to historical observations up to the year 2023 and are kept constant throughout the simulation period. The MAGICC7 model is calibrated to observations from the NOAA network for the historical period.

Surface methane concentrations for the CLE, MTFR, and HILO scenarios are available for download from Zenodo (van Caspel and Fagerli, 2025). It is important to note that the surface methane concentrations in each of the three scenarios are different. While the HILO scenario uses the same methane emissions as the CLE scenario, the resulting methane concentrations are not identical under CLE and HILO due to the different emissions of NO_x and NMVOC in these scenarios and the consequent effects on ozone, hydroxyl radical, and the methane lifetime.

For the Transient Historical experiment, historical concentrations of methane are also provided as annual average surface mixing ratio in van Caspel and Fagerli, (2025). For the historical period, these concentrations have been harmonised with the observations from the NOAA Global Monitoring Laboratory (Thoning et al., 2022). Modelling groups should fix the concentration of methane at their lower boundary to these values. Values are provided from 1998 to allow for up to five years of model spin-up.

5.6 Hydrogen

For all model experiments, groups must specify a global average surface mixing ratio of hydrogen of 530 ppb, equivalent to the present-day mixing ratio (Novelli et al., 1999). The GAINS LRTAP scenarios do not include emissions from a potential future hydrogen/ammonia economy, and other future projections of hydrogen emissions are too uncertain at this time.

5.7 Natural emissions and other emissions not specified in this experiment description

A key aim of the HTAP3-OPNS exercise is to minimise barriers to participation for modelling groups. As such, all modelling groups are free to choose whichever datasets are most convenient and appropriate for their model for natural emissions, and any other emissions not specified in this experiment description. We expect that each modelling group contributing to HTAP3-OPNS already has experience running their model and can make a judgement on the appropriate treatment of the emission sources and appropriate datasets required for their model simulations.

All groups are required to report their total emissions including both natural and anthropogenic emissions using the appropriate fields in the requested output data (Section 6) and additionally provide a description of the emission data sets or online calculations used for natural emissions or other emissions not specified in this experiment description in their simulations.

5.7.1 Emissions of Biogenic Volatile Organic Compounds

Each group is free to choose their own treatment of BVOC emissions. Ideally, BVOC emissions used in each model should be calculated online in a way consistent with the land cover and meteorology used in each model experiment, although we will also accept submissions from groups using offline BVOC emissions. Please note that reporting of both isoprene emissions and total BVOC emissions as model output fields are required in HTAP3-OPNS (Section 6).

5.7.2 Emissions of NOx from lightning

Each modelling group is free to choose their own treatment of lightning NOx emissions, including the overall magnitude of the lightning NOx source. Ideally, groups should use the same treatment of lightning NOx emissions as they have used in previously published evaluations of their respective models. Please note that reporting of lightning NOx emissions as a model output field is required in HTAP3-OPNS (Section 6).

5.8 Land cover

There is no requirement in HTAP3-OPNS to use any specific land cover treatment. Each modelling group is free to choose whichever land cover treatment is most appropriate and convenient for their model, as long as it is broadly consistent with the period being simulated in each model experiment (Section 7).

For an offline treatment of land cover, we recommend the use of the LUH2 dataset (Hurtt et al., 2020), which provides detailed land cover patterns from 850-2100, and was used by modelling groups contributing to the CMIP6 model intercomparison project.

5.9 Meteorology and climate boundary conditions

Modelling groups are free to choose whichever meteorological or climate input data is most appropriate and convenient for their model, within the constraints of the relevant experimental specifications (Section 7).

For CTMs contributing to the Perturbation and Transient Historical experiments, this input consists primarily of archived meteorological fields (specified dynamics) from a reanalysis product. HTAP recommends that CTM groups use meteorological input data which they have previously used in published evaluations of their respective models.

For CCMs contributing to the Transient Future experiments, this input consists of sea surface temperature and ice cover data, as well as the concentrations of well-mixed greenhouse gases (except for methane, which must be taken from the GAINS LRTAP scenarios as either emissions or concentrations, Section 5.5). Groups are free to choose whichever source of input data is most convenient for their model. HTAP recommends that CCM groups use input datasets for the historical period and SSP2-4.5 corresponding to their own CMIP6 simulations (or equivalent).

6 Requested model output data

The full list of requested model output fields for HTAP3-OPNS is available in the supplement to this manuscript. This HTAP3-OPNS output table is based on the requested output for AerChemMIP (Collins et al., 2017), with several modifications specific to HTAP3-OPNS. All modelling groups are encouraged to provide as many of the HTAP3-OPNS diagnostic fields as possible from their simulations for all sets of experiments in HTAP3-OPNS. Diagnostic fields of particular importance, as well as new fields which have been added for HTAP3-OPNS, are described in this Section below. A table of the full set of requested output fields is provided in the supplementary material to this manuscript. During drafting of this manuscript, the table is available here: https://nextcloud.gfz-potsdam.de/s/sp8XmMY2rQizjA4. There is a separate data request for regional models here: https://nextcloud.gfz.de/s/qaaTenoTeAPHctc. The format in which model output should be provided is described in Section 8.1.

For climate models contributing to the Transient Future experiments (Sec. 4.2 and 7.4), hourly fields should be saved in the first ten years (2010-2019) and last ten years (2040-2019) of each model run. All other models contributing to all other sets of experiments should save and report hourly fields for the full duration of each model experiment.

6.1 Hourly surface mixing ratio of ozone and other pollutants

In order to calculate policy-relevant ozone impact metrics, all groups are required to provide hourly averaged fields of the surface ozone mixing ratio at the lowest model level for all simulations in all sets of experiments. While this diagnostic was already included in the AerChemMIP output table, and is not new in HTAP3-OPNS, we emphasise the necessity of including this field for all models participating in all HTAP3-OPNS experiments.

In addition to the hourly mixing ratio of ozone, modelling groups are also strongly encouraged to provide hourly mixing ratio of PM2.5 and NO2 at the lowest model level, which will also be used in health impact assessment.

6.2 Ozone deposition and related fields

Ozone impacts on vegetation will be an important part of the analysis of HTAP3-OPNS. This will be jointly performed by HTAP in cooperation with ICP Vegetation (The International Cooperative Programme on Effects of Air Pollution on Natural Vegetation and Crops), a body of CLRTAP based at the UK Centre for Ecology and Hydrology. Ozone impacts on vegetation (primarily wheat crops and deciduous forests) will be determined using the PODyIAM (Phytotoxic Ozone Dose above threshold y for Integrated Assessment Modelling) metric using the DO3SE model (Emberson et al., 2007; Simpson et al., 2012).

Modelling groups who have implemented the DO3SE model (or equivalent methods for calculating the PODyIAM metrics) in their systems are encouraged to directly provide daily accumulated values of the relevant PODyIAM metrics. Crop impacts will be calculated from POD3IAM, and forest impacts will be calculated from POD1IAM. A detailed description for the calculation of these metrics is given in (CLRTAP, 2023). Groups who are able to calculate PODyIAM metrics should provide both POD1IAM and POD3IAM at daily resolution on a longitude/latitude grid.

All groups (including groups which calculate and provide the PODyIAM metrics) should provide hourly values of the following parameters (where available) as a high priority, which will be used to calculate the PODyIAM metrics offline:

- Hourly mean 2D (longitude, latitude) output:
    - Mixing ratio of ozone at the lowest model level (also requested in Section 6.1).
    - Ozone deposition flux.
    - Ozone deposition velocity.
    - Aerodynamic resistance as used in the deposition calculation.
    - Near-surface air temperature.
    - Near-surface relative humidity.
    - PPFD (Photosynthetic Photon Flux Density).

        - If this is not available, it can be calculated offline based on location and time.

- Daily mean 2D (longitude, latitude) output:
    - soil_moisture_content.
- Monthly mean 2D (longitude, latitude) output:
    - soil_moisture_content.
    - soil_moisture_content_at_field_capacity.
    - Land cover maps including all vegetation types used in the model runs.
    - Groups will also be asked to provide information about the land cover types used in their simulations.

Groups with the capacity to do so should also provide the soil_moisture_content variables at the vertical resolution of their soil model in addition to the vertically integrated soil moisture variables mentioned above (CF names moisture_content_of_soil_layer and moisture_content_of_soil_layer_at_field_capacity).

In addition to the requested data, all groups are also requested to provide detailed information about their ozone deposition schemes, in particular about whether and how soil moisture is included in the calculation of the deposition velocity.

6.3 Total deposition

The WMO MMF-GTAD exercise (https://community.wmo.int/en/activity-areas/gaw/science-for-services/mmf-gtad) requires comprehensive information on total atmospheric deposition. Modelling groups contributing to the HTAP3-OPNS experiments are encouraged to fully implement and provide these model diagnostics for all sets of experiments. Total deposition output is required for models contributing to the Transient Historical experiments, since this set of experiments will provide the model output for the MMF-GTAD exercise.

The requested deposition fields from the HTAP3-OPNS output table (monthly output) are as follows:

- dry deposition rate of O_3
- dry deposition rate of dry aerosol total organic matter
- wet deposition rate of dry aerosol total organic matter
- dry deposition rate of black carbon aerosol mass
- wet deposition rate of black carbon aerosol mass
- dry deposition rate of seasalt
- wet deposition rate of seasalt
- dry deposition rate of dust
- wet deposition rate of dust

- dry deposition rate of SO_2
- dry deposition rate of SO_4
- wet deposition rate of SO_4
- wet deposition rate of SO_2
- dry deposition rate of NH_3
- dry deposition rate of NH_4
- wet deposition rate of NH_4
- wet deposition rate of NH_3
- dry deposition rate of NO_y
- wet deposition rate of NO_y incl aerosol nitrate
- dry deposition rate of organic nitrate
- wet deposition rate of organic nitrate incl aerosol organic nitrate

Except for the deposition diagnostics for organic nitrates, all the requested deposition fields were already included in the AerChemMIP output tables. The organic nitrate deposition diagnostic fields were added to the HTAP3-OPNS output table at the request of the WMO MMF-GTAD exercise.

6.4 Ozone and other chemical budget terms

The ensemble of models contributing to the various sets of experiments of HTAP3-OPNS represents an opportunity to explore inter-model differences in ozone production and loss terms which may help to explain the inter-model differences in simulated ozone. Modelling groups with the capacity to provide chemical flux diagnostics are encouraged to provide appropriate output which can be used to construct detailed ozone budgets based on the approach described by (Edwards and Evans, 2017).

The AerChemMIP output tables already contain variables diagnosing the monthly mean ozone production and loss terms in units of $cm^{-3}s^{-1}$. For HTAP3-OPNS we ask for modifications to the ozone loss diagnostic, and several additional diagnostic fields to enable more detailed investigation of the ozone budget and comparison of tropospheric chemistry across participating models:

- The ozone loss diagnostic o3loss should be modified to include Ox loss due to halogen chemistry for models which include this chemistry.
- An additional diagnostic primo3loss is requested for primary ozone loss (as the tendency due to reaction between $O(^1D)$ and water vapour).
- Additional diagnostics do3chm and tropdo3chm are requested for the change in ozone across the chemical timestep.

- An additional diagnostic oxprodo2photo is requested for the production rate of Ox due to the photolysis of molecular oxygen.
- An additional diagnostic ohprod is requested for the total OH production rate, the OH production from all reactions producing OH, including rapid HOx interconversion..
- An additional diagnostic ohloss is requested for the total OH loss rate, the OH loss from all reactions consuming OH, including rapid HOx interconversion.
- An additional diagnostic prodco is requested for the secondary chemical production of CO.

The standard 2D diagnostics tropoz and toz are also requested as monthly averages. The variable toz is the total ozone column, while the tropospheric ozone column field (tropoz) is calculated using a dynamically varying online pressure tropopause (ptp) according to the WMO thermal tropopause definition. Both should be output on the model native lat/lon grid.

In addition to the extra diagnostic terms, we request all groups to provide a machine-readable file containing their model chemical mechanism to assist in the interpretation of the diagnostic terms. An overview of the planned analyses using these diagnostics is given in Section 8.2.6.

6.5 Boundary conditions for regional models

Since it will not be possible for HTAP to centrally host the large amount of data required for regional boundary conditions, data exchange between global and regional modellers should be organised directly between interested global and regional modellers. HTAP will help with coordination of this exchange. Further details on boundary conditions for regional modellers are given in Section 7.3.1.

6.6 Common radiation calls (for models with opportunities)

To quantify the effects of the individual emission components on the radiative budget we propose to include additional diagnostic double calls into the CCM model simulations. For aerosols we suggest applying the Ghan method (Ghan, 2013) and include an additional diagnostic ‘aerosol free’ radiation call. Similarly, we propose to include an additional diagnostic radiation call with an ozone climatology instead of the interactive ozone (see Collins et al. 2024). These double calls should be provided for instantaneous radiative forcing (IRF). Models which can also provide a stratospheric adjusted radiative forcing (SARF) are invited to provide these fields in addition. Modellers are encouraged to make this diagnostic output available to allow calculation of ERF as per CMIP6 protocol/experiments' for the ESM models.

7 Experimental setup

For all experiments in each of the three sets, participating modelling groups have the flexibility to configure their model as they see fit (e.g. grid resolution, meteorological/climate boundary conditions, natural emissions, chemical mechanism, etc…), as long as they adhere to the requirements for the use of specific input datasets as shown in Table 1 and described in Section 5, and provision of output fields described in Section 6.

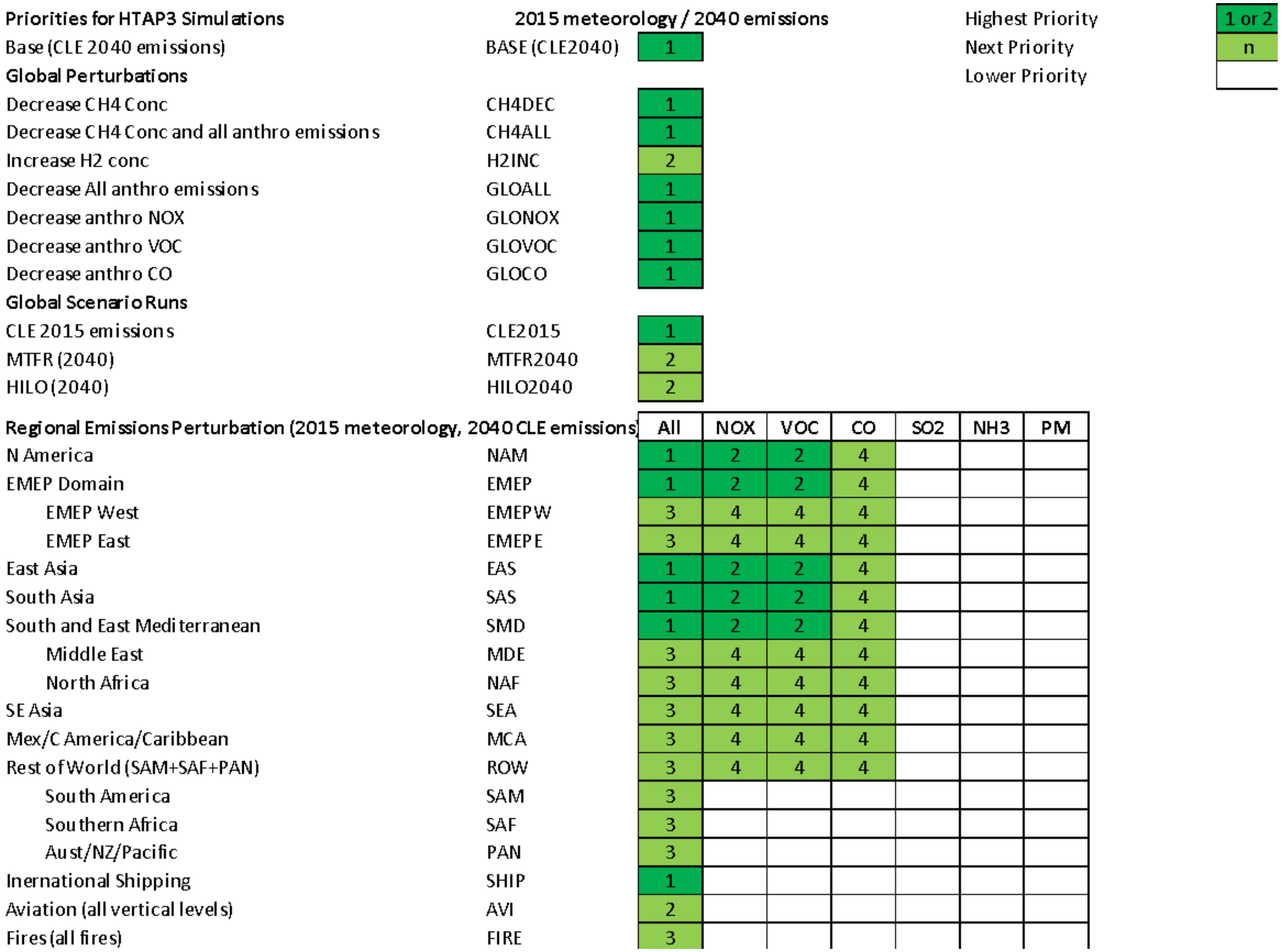
7.1 Perturbation experiments

All experiments in this set consist of year-long model simulations performed by global CTMs or CCMs with specified dynamics, land cover, biomass burning, and natural emissions for a common meteorological base year (2015). Anthropogenic emissions excluding agricultural waste burning for all model runs are based on GAINS LRTAP emissions (Section 5.1). Biomass burning emissions including agricultural waste burning are based on the GFAS4HTAP dataset (Section 5.3). Methane concentrations corresponding with the emissions from the three GAINS LRTAP scenarios (CLE, MTFR, and HILO, Section 5.5) are specified as concentration boundary conditions in all runs of this set of experiments. This set of experiments has two primary goals:

- Direct simulation of single years of the GAINS LRTAP scenarios (2015 and 2040) as a complement to the Transient Future experiments and for the provision of lateral boundary conditions to regional model simulations.
- Production of source/receptor relationships for hemispheric air pollution in 2040 for the construction of the HTAP3 ensemble emulator.

Model groups should ensure that their model is appropriately spun-up in each case. In general, we recommend at least 6 months of spin-up for each run (beginning in July and using the same emissions and meteorology as the simulation itself, if 2014 meteorology is not available for spinup then it is acceptable to use 2015 meteorology for the spinup), assuming that initial conditions are chosen appropriately, as recommended below. A good test for sufficient spin-up would be to compare the December output from the spin-up period with the December output from the delivered model output and to check for the absence of any chemical drift.

The runs in this set of experiments are shown in Table 3 and described in more detail below.



Priorities for HTAP3 Simulations	2015 meteorology / 2040 emissions	
Base (CLE 2040 emissions)	BASE (CLE2040)	1
Global Perturbations		
Decrease CH4 Conc	CH4DEC	1
Decrease CH4 Conc and all anthro emissions	CH4ALL	1
Increase H2 conc	H2INC	2
Decrease All anthro emissions	GLOALL	1
Decrease anthro NOX	GLONOX	1
Decrease anthro VOC	GLOVOC	1
Decrease anthro CO	GLOCO	1
Global Scenario Runs		
CLE 2015 emissions	CLE2015	1
MTFR (2040)	MTFR2040	2
HILO (2040)	HILO2040	2

Highest Priority	1 or 2
Next Priority	n
Lower Priority	

Regional Emissions Perturbation (2015 meteorology, 2040 CLE emissions)		All	NOX	VOC	CO	SO2	NH3	PM
N America	NAM	1	2	2	4			
EMEP Domain	EMEP	1	2	2	4			
EMEP West	EMEPW	3	4	4	4			
EMEP East	EMEPE	3	4	4	4			
East Asia	EAS	1	2	2	4			
South Asia	SAS	1	2	2	4			
South and East Mediterranean	SMD	1	2	2	4			
Middle East	MDE	3	4	4	4			
North Africa	NAF	3	4	4	4			
SE Asia	SEA	3	4	4	4			
Mex/C America/Caribbean	MCA	3	4	4	4			
Rest of World (SAM+SAF+PAN)	ROW	3	4	4	4			
South America	SAM	3						
Southern Africa	SAF	3						
Aust/NZ/Pacific	PAN	3						
Inernational Shipping	SHIP	1						
Aviation (all vertical levels)	AVI	2						
Fires (all fires)	FIRE	3						

Table 3 Overview of the perturbation experiments in HTAP3-OPNS.

All model runs should be performed using 2015 meteorology, biomass burning emissions, natural emissions, and land cover. Recognising that most modelling groups will not have the capacity to perform a large number of simulations, the model runs in Table 3 are prioritised according to their usefulness for constructing the HTAP3 ensemble emulator. There are 14 runs with a priority of 1, and another 10 runs with a priority of 2. Remaining runs are given either priority 3 or 4, or not requested at all. Construction of reliable model emulators requires contribution of results to priority 1 runs and would benefit from results for priority 2 runs; priority 3 and 4 runs provide useful additional information on regional and species contributions but are less essential.

All groups contributing simulations to this set of experiments are required to perform the base simulation, which uses GAINS LRTAP CLE 2040 emissions and methane concentrations, and another simulation using GAINS LRTAP CLE 2015 emissions and methane concentrations. The CLE2040 simulation will form the basis for all perturbation runs in this set, while the CLE2015 run will be used for model evaluation as well as to evaluate the change in global air quality between 2015 and 2040.

For the spin-up of the CLE2015 and CLE2040 simulations, we recommend initialising the model with archived 3D concentrations from an existing present-day simulation, but with 3D fields of methane and hydrogen set to the same values as the respective specified surface concentrations from each scenario. We recommend using the same initial conditions as CLE2040 for all other perturbation runs, except where otherwise specified. As mentioned above, we recommend six months of spin-up for each model run, but each group should ensure that their model is appropriately spun-up for each run.

7.1.1 Direct scenario experiments

There are four direct scenario runs requested in this set of experiments: CLE2015; CLE2040; MTFR2040; and HILO2040. These runs will be used to assess future global air quality under the GAINS LRTAP scenarios and as a source of boundary conditions for regional model simulations (Section 7.3.1).

The CLE 2015 and CLE 2040 runs have priority 1 because they are used respectively for model evaluation and as the base case for source/receptor runs. All groups contributing to the Perturbation experiments should perform these two runs.

The MTFR2040 and HILO2040 runs have priority 2 because they do not contribute directly to the construction of the HTAP3 ensemble emulator. However, global modelling groups providing lateral boundary conditions for regional model simulations should perform both of these runs as a matter of high priority. Other global modelling groups with additional resources and an interest in the assessment of these scenarios are also encouraged to perform these runs as long as they also perform the 14 priority 1 runs (Table 3).

For the spin-up of all direct scenario simulations, we recommend initialising the model with archived 3D concentrations from an existing present-day simulation, but with 3D fields of methane and hydrogen set to the same values as the respective specified surface concentrations from each scenario.

As noted in Section 3, all emission fluxes except for methane for the HILO scenario are taken from the MTFR scenario. As also noted in Section 5.5, methane concentrations for the HILO run in this set of experiments are calculated based on methane emissions from the CLE scenario, but the resulting methane concentrations are not identical between CLE and

HILO. Groups performing the HILO2040 run should take care to use methane concentrations from Met.no for the HILO scenario (Section 5.5).

7.2 Global perturbation experiments

Global perturbation runs are performed by decreasing the specified emissions or surface concentrations by 20% relative to the base run, as for previous HTAP assessments. There are six priority 1 global perturbation runs:

- CH4DEC: The global methane concentration boundary condition is reduced by 20%.
- CH4ALL: The global methane concentration boundary condition and all anthropogenic (including shipping and aviation) emissions (NO_x, NMVOC, CO, SO_2, NH_3, and all PM species) are reduced by 20% globally. Biomass burning emissions (including agricultural waste burning) and natural emissions are not changed.
- GLOALL: All anthropogenic (including shipping and aviation) emissions (NO_x, NMVOC, CO, SO_2, NH_3, and all PM species) are reduced by 20% globally. Biomass burning emissions (including agricultural waste burning) and natural emissions are not changed.
- GLONOX: All anthropogenic emissions (including shipping and aviation, but excluding agricultural waste burning) of NO_x are reduced by 20%.
- GLOVOC: All anthropogenic emissions (including shipping and aviation, but excluding agricultural waste burning) of NMVOC are reduced by 20%.
- GLOCO: All anthropogenic emissions (including shipping and aviation, but excluding agricultural waste burning) of CO are reduced by 20%.

In addition to the priority 1 global perturbation runs, there is also a priority 2 global perturbation run H2INC, in which the hydrogen concentration boundary condition is increased by 20%. Groups with the additional resources to perform this run are encouraged to do so, which will allow the HTAP3 ensemble emulator to include the atmospheric response to future changes in hydrogen.

For the CH4DEC and CH4ALL simulations, we recommend applying the 20% reduction in methane concentrations to the 3D initial conditions as well as to the surface boundary conditions to reduce the need for additional spin-up time. Similarly, for the H2INC simulation, we recommend applying the 20% increase in H_2 concentrations to the 3D initial conditions as well as to the surface boundary condition.

7.2.1 Regional and sectoral perturbation experiments

There are six priority 1 runs which include regional or sectoral emission perturbations of -20% relative to the base run of all anthropogenic species (NO_x, NMVOC, CO, SO_2, NH_3, and all PM species). The source regions for the perturbation experiments are shown in Figure 2 and are available for download from Zenodo (Butler, 2025). Please make sure to use version 4 of this dataset. Since the work has been designed to support the revision of the CLRTAP Gothenburg Protocol, the primary focus is the Northern Hemisphere. For the five regional perturbation runs, only the land-based anthropogenic emission sectors should be perturbed. No perturbation should be applied for aviation emissions, international shipping emissions, biomass burning emissions (including agricultural waste burning), or natural emissions.

- NAMALL: Emissions are reduced by 20% over the North American source region.
- EMEPALL: Emissions are reduced by 20% over the EMEP source region.
- EASALL: Emissions are reduced by 20% over the East Asia source region.
- SASALL: Emissions are reduced by 20% over the South Asia source region.
- SMDALL: Emissions are reduced by 20% over the Southern Mediterranean source region.

In addition to the priority 1 regional perturbation runs, we also request with priority 1 the SHIPALL perturbation run, in which all emissions from the international shipping sector (regardless of location) are reduced by 20%.

There are an additional 10 regional perturbation runs of priority 2 corresponding to the five major source regions with -20% perturbations of anthropogenic emissions (excluding aviation, all biomass burning sectors, and natural emissions) of individual pollutant species (5 NO_x perturbation runs and 5 NMVOC perturbation runs):

- NAMNOX and NAMVOC
- EMEPNOX and EMEPVOC
- EASNOX and EASVOC
- SASNOX and SASVOC
- SMDNOX and SMDVOC

For groups which have performed at least the 14 priority 1 runs (Table 3), and ideally also the 10 priority 2 runs, there are an additional 12 priority 3 regional or sectoral perturbation runs which would be of use in constructing the HTAP3 ensemble emulator:

- EMEPWALL and EMEPEALL: these runs help with disaggregation of the EMEP source region into its western and eastern parts.
- NAFALL and MDEALL: these runs help with disaggregation of the SMD source region into its component parts.
- ROWALL, SAMALL, SAFALL, and PANALL: these runs complete the coverage of all global source regions.
- AVIALL and FIREALL: these runs help to quantify the response of air pollution to emissions from aviation and biomass burning respectively.

Runs listed as priority 4 in Table 3 are useful in the construction of the HTAP3 ensemble emulator. Due to the large number of runs of priority 1, 2, and 3, we do not expect many groups to perform runs of priority 4. However, groups with a special interest in priority 4 perturbation runs are encouraged to perform these and submit them to the data archive if they have completed at least the 14 priority 1 runs, and ideally also the 10 priority 2 runs.

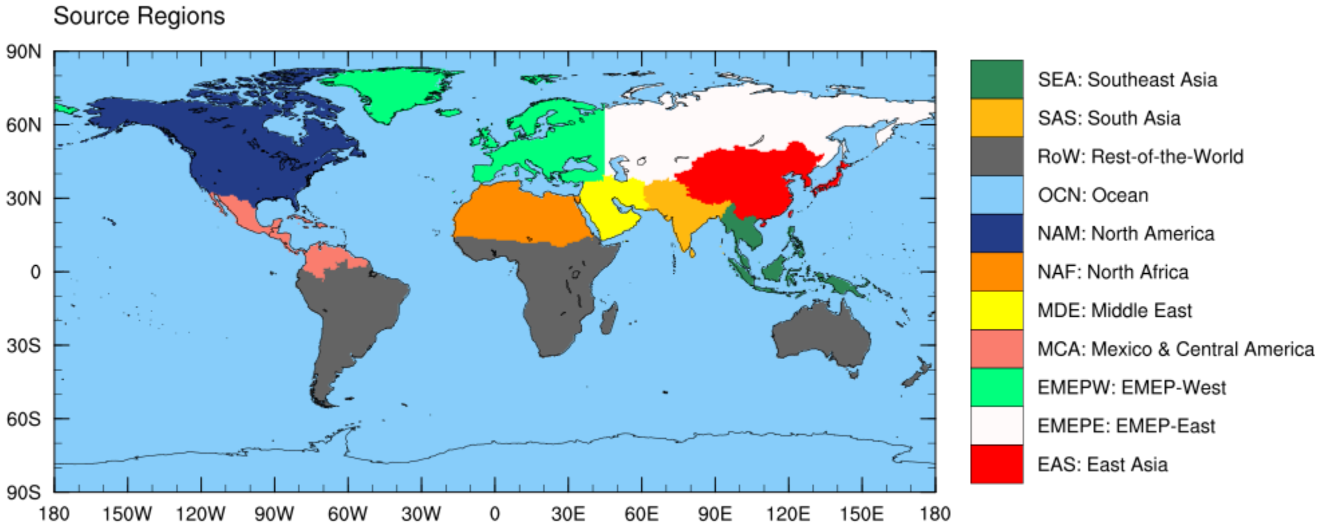


Figure 2 The HTAP3 source regions.

7.3 Global to regional downscaling of GAINS LRTAP scenarios

A major motivation for the work in HTAP3-OPNS is the revision of the CLRTAP Gothenburg Protocol, which regulates the emissions of ozone precursors and particulate matter in the UNECE region. Assessment of the GAINS LRTAP scenarios using high resolution regional models for Europe and North America is therefore an important part of HTAP3-OPNS. Depending on interest from regional modellers simulating other domains, there may also be demand for boundary conditions for other regions. For compatibility with global specified-dynamics simulations in HTAP3-OPNS, regional simulations should be performed using meteorological input from the common base year (2015).

7.3.1 Global simulations providing boundary conditions for regional models

Lateral boundary conditions for regional model simulations will be taken from the global simulations of CLE2015, CLE2040, MTFR2040, and HILO2040 (Section 7.1.1). Global modellers performing these four simulations are encouraged to save high temporal resolution output of key model species at high temporal resolution (at least 6 hourly) and 3D spatial resolution (or at the coordinates of regional model boundaries) in a format accessible for regional modellers. Given that HTAP will not have the resources to store these boundary conditions centrally on the AeroCom server, global modelling groups providing boundary conditions for regional models are requested to host these data themselves and make them available to regional modellers.

HTAP will make efforts to identify regional modellers interested in downscaling the GAINS LRTAP scenarios for their region using boundary conditions from HTAP3-OPNS global runs. HTAP will work to connect regional modellers with global modellers and help to identify the key species which must be saved from global simulations, and the coordinates at which these species should be saved.

NCAR will perform global simulations with the CAM-chem model and host global 3D 6-hourly output of the species listed here: https://wiki.ucar.edu/display/camchem/CESM+2.2%3A+Species+saved+in+boundary+condition+files. These species should be especially suitable for regional models using chemical mechanisms related to the MOZART mechanism as used in CAM-chem.

The CLRTAP MSC-W will perform global simulations with the EMEP model and host 6-hourly output at the edges of the CAMS and EMEP domains.

7.3.2 Regional model simulations for Europe

Several regional modelling groups with a focus on Europe have expressed an interest in performing simulations through fora such as the CLRTAP Task Force on Measurements and Modelling (TFMM) and the Copernicus Atmosphere Monitoring Service (CAMS).

European regional modellers are encouraged to perform simulations for the EMEP domain where possible, otherwise for the CAMS domain. Groups performing simulations using the CAMS domain must make sure to simulate the entire geographical extent of the CAMS domain.

All regional model input data should be harmonised as closely as possible with the descriptions given in Section 5. Meteorological input data should correspond with the base year (2015) for all simulations. Anthropogenic emissions excluding agricultural waste burning should be taken from the relevant GAINS LRTAP scenarios (Section 5.1).. Regional model simulations should not specify methane emissions within their simulation domain, but rather specify methane concentrations at their lateral boundaries. Biomass burning emissions including agricultural waste burning should be taken from the GFAS4HTAP dataset (Section 5.3) for 2015 for all simulations. Natural emissions should also correspond with the year 2015. All other aspects of model configuration are left to the discretion of the regional modelling groups.

A summary of the regional model simulations for Europe is given in Table 4. Five simulations are requested from each contributing modelling group. Simulations 1-3 use the same emission scenario in both the global and regional models. Simulation 4 uses MTFR emissions for air pollutants in both the global and regional domains and boundary conditions from the global HILO scenario. Simulation 5 uses boundary conditions from CLE2040, but emissions from all land-based anthropogenic emission sectors (excluding aviation and international shipping) in the EMEP West source region (Figure 2 and Butler et al., 2025) within the regional model domain are replaced with the corresponding emissions from the MTFR2040 scenario. All regional simulations should cover the full meteorological year 2015.

Simulation number	**Simulation name**	**Emissions in the EMEP West region**	**Emissions in all other regions**	**Boundary conditions from global model**
1	CLE2015	CLE2015	CLE2015	CLE2015
2	CLE2040	CLE2040	CLE2040	CLE2040
3	MTFR2040	MTFR2040	MTFR2040	MTFR2040
4	HILO2040	MTFR2040	MTFR2040	HILO2040
5	EMEPWLO2040	MTFR2040	CLE2040	CLE2040

Table 4 Regional model simulations for Europe in HTAP3-OPNS

It is anticipated that several different sets of boundary conditions from different global models will be available for these simulations (Section 7.3.1). Regional modelling groups are free to choose the most convenient dataset, and encouraged to choose the global model output which most closely corresponds to their chemical mechanism. Groups with the resources to perform additional simulations are encouraged to perform the same set of five regional simulations using alternative boundary conditions.

Regional modelling teams should format their model output according to the instructions in Section 8.1 before uploading their data to the AeroCom server, taking care to include the fields which are indicated to be of high priority for HTAP3-OPNS.

7.4 Transient future experiments

In this set of experiments, transient model simulations will be performed by CCMs with the GAINS LRTAP scenarios (Section 5.1) from 2010-2050 and the future fire emissions described in Section 5.2. The 10-year period 2010-2019 will be used to determine the baseline conditions for the present day (corresponding to the year 2015), and the 10-year period 2040-2049 will be used to determine the conditions corresponding to the end of the scenarios. The full transient timeseries of model output will be used to determine the model responses to changing emissions.

7.4.1 Scenarios and prioritisation

All CCM groups contributing to the Transient Future Scenarios experiments are requested to run at least the three core scenarios: CLE; MTFR; and HILO, as described in Sections 3 and 5.1. All three of these scenarios should be run with climate forcing corresponding to SSP2-4.5. Comparison of these three scenarios with each other will directly inform the Gothenburg Protocol revision process with an understanding of future air quality under these three emission pathways. In addition to the three core scenarios, CCM groups with the resources to run an additional three simulations are requested to run the same three core emission scenarios, but with constant fixed climate forcing corresponding to the year 2015. Comparison of the fixed 2015 climate forcing simulations with the transient-forcing SSP2-4.5 simulations will allow calculation of the climate penalty on air pollution under the GAINS LRTAP scenarios.

Modelling groups with the capability of performing methane emissions-driven simulations are strongly encouraged to do this for their contributions to the Transient Future Scenarios experiments. Surface methane mixing ratios for concentration-driven model runs are described in Section 5.5). As noted in Section 5.5, the methane concentration pathways in each of the three scenarios are distinct. Groups may submit both emissions-driven and concentration-driven simulations for each scenario if they wish. A summary of the six requested runs is given in Table 5.

Run name	**Priority**	**Transient emissions scenario, including methane trajectory**	**Climate forcing**	**Radiation coupling**
ssp245-CLE-CH4conc **OR** ssp245-CLE-CH4emis	1	GAINS LRTAP CLE	SSP2-4.5 transient	Fully coupled with composition
ssp245-MTFR-CH4conc **OR** ssp245-MTFR-CH4emis	1	GAINS LRTAP MTFR	SSP2-4.5 transient	Fully coupled with composition
ssp245-HILO-CH4conc **OR** ssp245-HILO-CH4emis	1	Hybrid scenario HILO	SSP2-4.5 transient	Fully coupled with composition
clim2015-CLE-CH4conc **OR** clim2015-CLE-CH4emis	2	GAINS LRTAP CLE	Constant 2015	Decoupled from composition (no ARI/ACI, all aerosol and GHG forcing fixed at 2015 composition, radiation sees a 2015 stratosphere)

clim2015-MTFR-CH4conc **OR** clim2015-MTFR-CH4emis	2	GAINS LRTAP MTFR	Constant 2015	Decoupled from composition (no ARI/ACI, all aerosol and GHG forcing fixed at 2015 composition, radiation sees a 2015 stratosphere)
clim2015-HILO-CH4conc **OR** clim2015-HILO-CH4emis	2	Hybrid scenario HILO	Constant 2015	Decoupled from composition (no ARI/ACI, all aerosol and GHG forcing fixed at 2015 composition, radiation sees a 2015 stratosphere)

Table 5 Chemistry-climate model simulations for the Transient Future experiments in HTAP3-OPNS

7.4.2 Chemistry-climate model setup

Groups are encouraged to use any version of their model which they think is appropriate, although we recommend that they use their CMIP6-AMIP configuration. Model output of the fields described in Section 6 in the format described in Section 8.1 should be reported for the years 2010-2050, with the exception of hourly surface fields, which should only be reported for the first ten years (2010-2019) and last ten years (2040-2049) of each model experiment. Model runs should begin from a sufficiently spun-up state in the simulation year 2010. We leave the details of model spin-up to each modelling group.

7.4.3 Climate forcing data

Climate forcing data for each run consists of the following fields:

- Sea surface temperatures.
- Ice cover.
- Land cover (unless using a dynamic land model).
- Concentrations of long-lived greenhouse gases (except for methane, which should be specified from the GAINS LRTAP scenarios).
- Ozone depleting substances.

For the “ssp245” runs, the climate forcing fields should be taken from the CMIP6 SSP2-4.5 forcing data. Fields not directly specified in SSP2-4.5 (SST and ice cover data) could be taken from a previous run of a fully coupled ESM forced with SSP2-4.5. As the SSP2-4.5 forcing data begins in 2015, modelling groups will need to perform the first part of their ssp245 simulations up until 2014 (including the spin-up) with historical forcing data. We recommend that groups begin their spin-up by branching from an existing CMIP6 historical simulation of their model, substituting the GAINS LRTAP scenarios from the branching year. The choice of branching year for sufficient spin-up is left to the judgement of each modelling group.

For the “clim2015” runs, the climate forcing fields, CO2 concentrations, other long-lived GHG (apart from methane), and ozone depleting substances should be taken from the year 2015 of an appropriate SSP2-4.5 dataset and kept constant throughout the entire simulation (including sufficient spin-up). All aspects of radiative forcing should also be kept constant at 2015 levels; this means that the evolving simulation of atmospheric composition (including methane, ozone, particles, and stratospheric composition) in response to the GAINS LRTAP scenarios should be decoupled from the model radiation scheme in the clim2015 simulations, with the model radiation seeing 2015 composition.. Fields not directly specified in SSP2-4.5 (SST and ice cover data) should be taken from a 10 year (2005-2014) average of a previous fully-coupled historical run of a fully coupled ESM. Land cover data should be kept constant in the clim2015 runs.

We note that the updated versions of the GAINS LRTAP scenarios will diverge from one another from the year 2025. Where appropriate, modelling groups are advised to branch their future simulations from this year to save storage and computational resources.

7.5 Transient historical experiment

This run should be performed with specified dynamics, the HTAPv3.2 global mosaic anthropogenic emissions (Section 5.4), the GFAS4HTAP biomass burning emissions (Section 5.3), and surface methane concentrations from the NOAA network (Section 5.5) for the period 2003-2020. Groups not in the position to perform the full time series should focus on the latter part of the period and include at least the year 2015 in their simulation. Groups performing this simulation are required to include total deposition output in their data submission (Section 6.3), as this will be provided to the WMO MMF-GTAD exercise.

8 Data handling

8.1 Initial delivery of data

Model output from HTAP3-OPNS as specified in the data request (Sec. 6) will be stored on the AeroCom server (https://aerocom.met.no). All groups contributing model output to HTAP3-OPNS must request an account on this server linked to the HTAP3-OPNS project. Data must be uploaded to the AeroCom server on a regular lat/lon grid. Model grids based on other projections or unstructured grids should be regridded by each modelling group to a regular lat/lon grid before being uploaded to the AeroCom server.

Data must be submitted in the CF-compliant netCDF format with file names based on the following convention:

- htap3opns_<ModelName>_<ExperimentName-PerturbationRealisation>_<DataRequestSheet>_<VariableName>_<Period>.nc

Where:

- <ModelName> should be chosen such that model name, model version, and possibly the institution can be identified. No underscores (_) are allowed in <ModelName>, use (-) instead. Restrict <ModelName> to max 20 characters.
- <ExperimentName> = will either be TransientHistorical, or follow the naming conventions introduced for each experiment in Sections 7.1, 7.3, and 7.4. For the various emissions perturbation runs, PerturbationRealisation will be 5-8 letters (3-5 indicating the region of perturbation and 2-3 indicating the pollutants or sector decreased) based on the experiment matrix in Table 3. For example, CLE2040-GLOALL is used to indicate a 20% decrease in anthropogenic emissions globally; CLE2040-NAMNOX is used to indicate a 20% decrease in anthropogenic NOx emissions from North America; and CLE2040-EMEPWVOC is used to indicate a 20% decrease in anthropogenic NMVOC from the EMEP West region.
- <DataRequestSheet> refers to the name of the sheet in the data request in which the variable was requested = aerfixed, aermonthly-3d, aermonthly-2d, aerdaily, aerhourly, aerzonal-vert, aerzonal, ModelLevelAtStations.
- <VariableName> = are the HTAP variable *short* names in the requested output spreadsheet discussed in Section 6 above. An example of a variable *short* name is: vmro3
- <Period> = year of simulation, corresponding to the meteorological year

8.2 Analysis of model experiments

During the analysis phase of HTAP3-OPNS, access to the submitted model output will be restricted to users of the AeroCom server who have requested access to the HTAP3 project. Groups who have not contributed model output, but who are interested in contributing to the analysis are welcome to contact the HTAP leadership team. The HTAP leadership team will organise regular meetings during 2025-2026 for all participants in the project to gauge the progress of model simulations and to coordinate the associated analyses. A non-exhaustive summary of some expected analysis is given below in this Section.

8.2.1 Model evaluation

Comparison of model results with observations is vital for determining the degree to which models are capable of simulating the historical past and providing confidence in their ability to make future projections. The requested model output fields in HTAP3-OPNS (Section 6) include hourly surface (2D) values of ozone, NO_2, PM_{10}, $PM_{2.5}$, and other species which are routinely measured at surface sites. With its focus on the impacts of air pollution on human health and ecosystems, the evaluation of model results against surface observations will be of high priority. In addition to hourly surface concentrations, the requested model output also includes other fields which can be used in model evaluation, such as Aerosol Optical

Thickness (AOT) at different wavelengths, deposition fields, and monthly mean 3D concentrations. Results from the CLE2015 CTM experiment (Section 7.1.1), the first 10 years of the transient future experiment (Section 7.4), and the full transient historical experiment (Section 7.5) will deliver output suitable for evaluation.

8.2.2 Source-receptor relationships and emulator development

The source-receptor relationships from the perturbation experiments (Section 7.1) will allow the construction of an ensemble emulator for rapid assessment of alternative future emission scenarios. Previous HTAP assessments have demonstrated the value of this approach for quantifying surface concentration changes across a wide range of future scenarios along with an estimate of the associated uncertainty as represented by the spread of responses across contributing models (Turnock et al., 2018; Wild et al., 2012). The approach allows incorporation of the nonlinearity in model responses and provides a valuable tool to guide policy development. Use of a 2040 baseline will allow exploration of source-receptor relationships under future conditions, permitting a more robust assessment of the effectiveness of mitigation measures around this policy-relevant target year. Groups are encouraged to submit results for as many of the runs as they can, but to focus in particular on runs defined as high priority to permit reliable emulation of their model.

8.2.3 Assessment of future air quality

An assessment of the air quality under the GAINS LRTAP future scenarios is a fundamental goal of HTAP3-OPNS. The transient future experiments (Section 7.4) will provide a direct assessment of future air quality using state-of-the-art Chemistry-Climate Models both with and without the effects of climate change. The direct scenario experiments (Section 7.1.1) will add to this with Chemical Transport Model simulations of air quality in 2040. The CTM ensemble emulator (Section 8.2.2) will also allow the attribution of future air quality to specific source regions. Analyses of future air quality using results generated in HTAP3-OPNS will be coordinated by TF-HTAP and a synthesis report will be written by the TF-HTAP leadership team for presentation to the Convention on Long-Range Transboundary Air Pollution.

8.2.4 Ozone impact on health

The collection of hourly surface ozone mixing ratio from all participating models (Section 6.1) will allow the calculation of health impact metrics based on the MDA8 (Maximum Daily 8-hour Average) ozone mixing ratio at the year and seasonal levels to compute the appropriate exposure indicators (e.g. peak season ozone, SOMO35). Such metrics will be used to estimate premature mortality, years of life lost attributable and other health outcomes attributable to ozone exposure by means of concentration-response functions (Huangfu and Atkinson, 2020; Murray et al., 2020, Kasdagli et al., 2024) associated with all-cause or specific causes of mortality (e.g. respiratory disease or chronic obstructive pulmonary disease). In this way it will be possible to link the measures and assumptions in the studied scenarios, especially those concerning the influence of methane emissions on ozone concentrations, with their implications for health. The information about regional emissions and activity sectors will be used to provide insights about the allocation of health impacts to their sources (Belis and Van Dingenen, 2023). In addition, the health impacts of other pollutants such as $PM_{2.5}$ and NO_2 and their implication for this analysis will be also explored.

8.2.5 Ozone impact on vegetation

This analysis was briefly introduced in Section 6.2. HTAP and ICP Vegetation will calculate the PODyIAM metrics using a standardised land cover dataset. The land cover provided by the modelling groups will be used to better understand the provided deposition fluxes and as a consistency check with the standardized dataset used by ICP Vegetation. This calculation will also use the provided hourly temperature, humidity, and PPFD where available. The availability of daily average soil moisture output will provide additional flexibility for the PODyIAM calculation. Impacts of ozone deposition on vegetation co-occur with effects of changing climates (e.g., higher temperatures and in some regions more frequent and intense drought events). The proposed simulations will allow us to unravel interactions between changing climatic conditions and ozone deposition and their impacts on vegetation.

8.2.6 Ozone budget analysis

Several analyses are planned using the additional chemical diagnostics requested in Section 6.4. The addition of halogen loss reactions for ozone will help with closing the ozone budget. The addition of the primary ozone loss term will help to separate the role of model physics (this is driven by photolysis) from the role of model chemistry in ozone loss. The addition of the OH production term will enable comparison of primary and secondary OH production across models (the primary OH production is equal to the primary ozone loss) and thus provide insight into inter-model differences in chemistry. The addition of the OH loss term enables calculation of the OH lifetime, which can be compared with available measurements, for example from the ATom field measurements (Wofsy et al., 2018).

8.2.7 Climate forcing of air pollution

The CLRTAP Gothenburg Protocol controls emissions of PM and ozone precursors over large parts of the UNECE region in order to improve air quality. These pollutants, along with methane, which is being considered for inclusion in the revised Gothenburg Protocol also exert a radiative forcing on the climate system. The model experiments in HTAP3-OPNS will allow the calculation of the radiative forcing due to these air pollutants, providing CLRTAP with information on the expected climate impact of potential future emission control measures.

8.2.8 Deposition of air pollutants

Detailed fields of total atmospheric deposition are requested in all experiments under HTAP3-OPNS, allowing interested groups to perform their own analyses. In particular, the deposition fields requested from the transient historical runs (Section 7.5) will be used in the WMO MMF-GTAD (Measurement-Model Fusion for Global Total Atmospheric Deposition) along with available deposition measurements to produce deposition maps of nitrogen, sulphur, and ozone (Fu et al., 2022).

8.3 Archiving of data

Once the initial set of analyses is completed, the access to the HTAP3 data on the AeroCom server will be opened up to any user with an account on the server. Due to the expected large volume of raw model output stored on the AeroCom server, permanent archiving of the full set of contributed data is not feasible. Permanent archiving of subsets of the contributed data which have been used in the production of scientific publications will be a condition of using data from HTAP3-OPNS in scientific publications. Suitable data repositories with version control and the assignment of DOIs include Zenodo (https://zenodo.org) and GFZ Data Services (https://dataservices.gfz-potsdam.de/portal/).

9 Links with other multi-model activities

9.1 HTAP1 and HTAP2

The design of the perturbation runs will be based on the experience gained during previous HTAP multi-model exercises. It will be important to limit the number of perturbation runs (source regions and emitted species) so that modelling groups are not overwhelmed by the number of runs to perform. The design of the perturbation runs is being done in close cooperation with the group responsible for the development of the ensemble emulators to ensure that the ensemble emulator is as useful as possible.

An important difference between the HTAP3-OPNS set of runs and previous HTAP multi-model assessments will be a focus on policy-relevant ozone metrics. Whereas in previous HTAP assessments, most models delivered monthly mean fields, in HTAP3 we will be asking for hourly mean surface (2D) fields of ozone mixing ratio and deposition fluxes. These hourly surface fields are required in particular to allow the calculation of the impacts of ozone on vegetation and will also enable more flexible and consistent calculation of human health impact metrics.

9.2 HTAP3-Fires and IGAC BBurned

To avoid duplication of work and to provide as large a set of model runs as possible for both projects, the base runs in the HTAP3-OPNS set are being harmonised as much as possible with the work being co-organised with the IGAC BBurned activity (Whaley et al., 2024):

- Common (or overlapping) base years for historical simulations.
- Use of the HTAPv3 anthropogenic emissions.
- Use of the same historical and future fire emission datasets.

The HTAP3-Fires activity is expected to continue well beyond the 2024-25 CLRTAP workplan, while HTAP3-OPNS is expected to be largely completed by 2026.

9.3 MCHgMAP

Where possible, model runs done for MCHgMAP (Dastoor et al., 2024) will be set up as closely as possible to the HTAP3-OPNS set of runs. A priority here will be the use of common fire activity data between MCHgMAP, HTAP3-Fires, and the HTAP3-OPNS runs.

9.4 AerChemMIP and CCMI

We invite participation from the chemistry climate modelling community using models with interactive tropospheric chemistry and aerosols for the simulation of future emissions scenarios. Modelling groups are requested to use their CMIP6 model configurations with fixed SSTs based on SSP2-4.5 for simulations of the LRTAP CLE and MTFR future emission scenarios.

9.5 MethaneMIP

There is some small overlap between the future scenario CCM runs requested in the HTAP3-OPNS set and work being planned under MethaneMIP (https://wcrp-cmip.org/mips/), as both efforts include an analysis of methane mitigation measures. Based on the current planning for both exercises however, this overlap does not warrant merging both activities.

A primary objective of MethaneMIP is to isolate the climate impact of methane mitigation, with air quality impacts being a secondary objective. MethaneMIP builds on the existing SSP2-4.5 base runs that modelling groups have already performed for CMIP6. This determines the MethaneMIP experimental design of fully coupled (including oceans) transient sensitivity runs with only methane being changed from the SSP2-4.5 base case.

In contrast, HTAP3-OPNS aims to perform an assessment of air quality under the GAINS LRTAP future emission scenarios, including the effects of all precursor emission changes (including methane but also NO_x, NMVOC, etc…) and the effects of the changing climate on the air quality response. This determines our experimental design, which only calls for prescribed SSTs and CO_2 forcing from SSP2-4.5 (CLE and MTFR scenarios) in the transient free running cases.

10 Summary

The HTAP3-OPNS multi-model exercise has been designed by the Task Force on Hemispheric Transport of Air Pollution (TF-HTAP) to provide scientific input to the Convention on Long-Range Transboundary Air Pollution (CLRTAP) in support of the current revision of the Gothenburg Protocol, the CLRTAP protocol to abate acidification, eutrophication, and ground-level ozone. Using an ensemble of Chemical Transport Models and Chemistry-Climate Models, along with future emission scenarios specifically developed to support the revision of the Gothenburg Protocol, this exercise will deliver information on the long-range (intercontinental) transport of multiple pollutants across the Northern Hemisphere.

Building on previous assessments by TF-HTAP, a major focus of this exercise will be ground-level (tropospheric) ozone. Results from the exercise will inform CLRTAP about the relative contributions of locally emitted ozone precursors and ozone precursors emitted in remote source regions to the impacts of ground-level ozone on human health and ecosystems, both inside and outside the UNECE region. These results will inform CLRTAP on options for mitigation of ground-level ozone through controls on emissions of ozone precursors, including controls on methane emissions. In addition to the usefulness for policymakers, the results from this study will deliver information about the suitability of current models for quantifying ground-level ozone and its impacts and point the way to future model improvements.

A set of perturbation simulations using Chemical Transport Models and pre-existing emission scenarios will allow the construction of detailed source/receptor relationships which will be used to develop an ensemble emulator, which will be used to explore mitigation options in more detail. Transient simulations with Chemistry-Climate Models will be used to explore the impact of climate change on future air quality under policy-relevant air pollution control scenarios. Simulations of the recent historical period using a state-of-the-art global mosaic emission inventory will aid in model evaluation and provide a basis for connecting this exercise with other concurrent exercises focusing on total atmospheric deposition and the impact of wildfires on air quality. The HTAP3-OPNS multi-model exercise is open to all interested modelling groups, and all other groups wishing to contribute to the analysis of model output datasets.

11 Data availability

All of the required model input datasets for HTAP3-OPNS are freely available as described in Section 5. Model output data will be published as described in Section 8; model output (as delivered by modelling groups, Sec. 8.1) will be made available to all groups interested in contributing to analyses after registration, and output datasets used in the production of scientific publications will be permanently archived with version control and DOIs assigned.

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