Project: **1395**

Project title: **Numerical modelling for transport research**

Principal investigator: **Johannes Hendricks**

Report period: **2024-11-01 to 2025-10-31**

Summary

Experiment	Status
Response model aerosol	**Conducted, except for cuts:** Using more than the allocated resources until the end of 2024, we performed all planned perturbed parameter ensemble (PPE) training simulations with aerosol and precursor emission variations. Three further regions were targeted for the radiative effects of land-based transportation emissions.
Response model gas phase	**Conducted completely:** An EMAC configuration for international shipping PPE training simulations with O_3 precursor emission variations was developed, tested, and applied for one region.
Hydrogen: chemistry and radiation	**Conducted partially:** The base configuration of EMAC for the simulations for the Horizon Europe project HYway was developed, tested, and applied in a 2010–2019 chemistry evaluation simulation.
Hydrogen: soil sink	**Conducted partially:** EMAC was extended to read in external deposition velocities. A setup that reproduces currently observed H_2 surface concentration when adding H_2 emissions was developed and applied.
Data experiments	**Conducted partially:** While "**Data: Response model aerosol**" was and is used for further developments of the methodology, for "**Data: Transport effects on gas phase chemistry**" we decided against the re-archival of the 130 TiB that we had applied for, and kept our focus on the SSP-based analyses.

Detailed report

Experiment "Response model aerosol"

In order to develop aerosol response functions for the climate response model TransClim (Rieger and Grewe, 2022), a large number of emission variation simulations has been performed to characterize the aerosol radiative forcing as a function of anthropogenic emissions of four aerosol and aerosol precursor species, namely nitrogen oxides (NO_x), sulfur dioxide and sulfate (SO_x), black carbon (BC), and organic carbon (OC). As before, we used the Righi et al. (2023) EMAC configuration for these simulations.

For emissions from land-based sources, aerosol response functions for three regions of interest were missing after the last reporting period: North America, South America and the "Rest of the World". We employed our new approach developed during the previous reporting period, namely that of a perturbed parameter ensemble (PPE), to also perform training simulations for these three regions.

For each region, our PPE requires 40 emission scaling factor combinations, which are sampled evenly from the four-dimensional parameter space using the Latin Hypercube method. The evaluation of the derived response functions against prior EMAC simulation results showed that it was useful to include an additional sampling point with emissions of all four species set to zero. Hence, a total of 123 simulations of 11 years each were performed during this reporting period.

Although we began the simulations using additional unallocated resources towards the end of 2024, the 200 planned simulations for the clean background could not be realized with the granted computing time.

Experiment "Response model gas phase"

For the extension of TransClim's gas phase component to include international shipping, we combine the method developed by Rieger and Grewe (2022) with the PPE approach described above for the aerosol component. This means running training simulations with EMAC in quasi chemistry transport mode (QCTM) with the sub-model TAGGING to track contributions of ship emissions to ozone concentrations and methane lifetime. Due to very small meteorology effects on the annual means of these contributions, simulations can be much shorter than in the aerosol case.

To obtain an up-to-date version of this EMAC configuration, many test simulations have been conducted in Q2/2025. Starting from Q3/2025, four candidate reference runs of three years each were carried out and systematically evaluated for "present-day" conditions (year 2015). One of them was chosen as the basis for the PPE simulations. For the gas phase effects, the varied emissions include only three species: NO_x, volatile organic compounds (VOCs), and carbon monoxide (CO). Therefore, our ensembles here consist of 30 different combinations of emission scaling factors for the training, and we added three combinations for verification. Thus, in total, 33 simulations are required to train and test our Gaussian process regressor for each region in which we vary the emissions. To save computing resources, we only run these simulations for 1.5 years each. During the current reporting period, we performed the 33 simulations for one region, namely the global oceans as a whole.

In order to also save disk and archive space, we decided to store only monthly mean output of these simulations, in contrast to the 5-hourly output, with which we had planned. Besides the fewer conducted simulations than planned in the following two experiments, and the reduced requirements of /arch space mentioned in the summary of the Data experiments, this is the main reason why we have used much less space on /work/bb1395 and /arch/bb1395 than what we applied for.

Experiment: "Hydrogen: Chemistry and radiation"

This experiment is part of the EC-funded project HYway that aims to reduce the uncertainties associated with the climate effects of additional H_2 in the atmosphere. Due to loss of personnel, a serious bug that required many test simulations to be found and fixed, and major adaptations of the setup (starting from RD1-base-01 from DKRZ project 853) being required for the HYway project simulations, the first 11-year production simulation could only be started in August. It is a transient simulation of the years 2010-2019 with one year of spin-up, meant to evaluate the H_2-related chemistry. The output data was further processed and shared with the project partners during September and October.

The H_2 emissions and CH_4 surface concentration perturbation simulations, for which we had also requested resources, will be started soon. While the reference run for these simulations is about to be finished (see next section), the sectoral perturbations, for which we had requested further resources, require more detailed planning within the HYway consortium and are now planned for 2026.

Experiment "Hydrogen: soil sink"

An accurate simulation of present and future H_2 emissions effects requires a dynamic representation of the main H_2 sink, namely the soil sink, which we aim to implement for EMAC in T42 resolution. With the model setup from the above experiment becoming available later than expected, and longer queuing times due to the cut on the requested computing time, we were not able to finish all the tasks originally envisaged for this experiment in 2025.

In support of the Horizon Europe project HYway, and in order to have a reference for the simulations with a fully dynamical, parameterized H_2 soil sink, we implemented the ability to read in externally supplied deposition velocities into EMAC. We tested this setup, including H_2 emissions, with several short simulations, and tuned the deposition velocity to arrive at observed present-day H_2 surface concentrations, as required by the simulation protocol of the HYway project. This simulation will serve as the reference for the perturbation simulations for the above experiment.