Project: **1393**

Project title: **Global aerosol modelling for transport and aviation research**

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Report period: **2025-11-01 to 2026-10-31**

The planned scientific work in Project 1393 during 2026 was focused on five main scientific topics. Several of the planned activities could not be fully carried out as intended, due to a significant cut in allocated resources. Approximately 10% of the resources were not consumed in Q3, due to a prolonged DKRZ maintenance caused by the file system issue at the end of August and the subsequent machine overload in September, which resulted in waiting times longer than usual in Slurm. With the continuation of the planned activities in Q4, we expect to consume the remaining budget of about 32 000 CPU node-h.

1. Training simulations for an aerosol response model

Most of the planned simulations for developing the aerosol response model and targeting the shipping sector could be performed as planned, with some adjustments to the original plan, following the results of a preliminary analysis. In this preliminary analysis, five different ocean regions were considered (open ocean and four coastal regions) to investigate the climate effects of shipping in different world regions with distinct emission characteristics. A subset of 5 PPE experiments has been performed for the two largest regions and for a macro-region combining all coastal regions. Statistical significance tests were applied to check whether a statistically significant effect could be extracted from these experiments. As the results were not statistically significant, the original plan was redefined and PPE experiments targeting the shipping sector at the global level were performed instead. These include a further study considering a clean background scenario based on SSP1-1.9. The latter set of experiments has been conducted twice to investigate the impact of updating methane boundary conditions in the clean background scenario. Furthermore, the PPE simulations targeting the land-based anthropogenic sector performed in the last reporting period have been extended by 4 test simulations for each of the 5 land regions to evaluate the regional emulators generated with Gaussian process regression. The resulting emulator will be documented in a publication currently in preparation.

2. Further development of the aerosol response model

The originally planned simulations for the improved aerosol response model could not be performed, partly due to resource cuts, but also because the model configuration took longer than expected. It was decided to use a more recent version of EMAC rather than the version used in Righi et al. (2023), as it features several important improvements that are useful for the development of the aerosol response model. In particular, the new version includes a model fix that resolves a restart-frequency-dependency issue in nudged mode, which would have prevented running the model in QCTM mode as planned. We also decided to use the newer PSrad radiation scheme, as opposed to the ECHAM5 radiation scheme used so far, since it is considered more advanced (Nützel et al., 2024). This required a re-tuning of the model. Given the experience gained in this project with the PPE approach (see Sect. 1), we also decided to apply it for tuning purposes. We designed an ensemble of tuning experiments targeting 6 tuning parameters, based on previous approaches with EMAC (Righi et al., 2020; Nützel et al., 2024). We drew 60 samples from the 6-dimensional parameter space using Latin hypercube sampling and performed a short (3-year) simulation for each sample. We used these points to train an emulator to cover the entire parameter space for a series of target cloud and radiation variables. This allowed us to emulate the values of these variables over the whole 6-dimensional space and compare them against observations. By minimizing the bias between model and observations (in terms of globally averaged values), we finally derived the best combination of the 6 parameters to be used for tuning. We are now finalizing this tuned configuration using the new model version. This can then be applied to the development of the aerosol response model and to other studies with EMAC in the aerosol-cloud-coupled setup, as proposed for the next reporting period.

3. Global aerosol dataset in support of life-cycle modelling for aircraft engines

During the previous collaboration between DLR and Rolls-Royce Deutschland, we provided atmospheric data for the period 2001–2024 to support life-cycle analysis of aircraft engines at Rolls-Royce Deutschland. We also applied a machine-learning-based clustering method to identify different aerosol regimes in the troposphere and lower stratosphere, as a more efficient approach to drive engine life-cycle models with a reduced-size dataset. Due to a funding reduction on the project partner's side, the project end has to be

moved up to 2026. The activity planned for the reporting period to further extend the atmospheric data to 2025 was therefore not carried out.

4. Improved representation of secondary organic aerosol particles

Simulations with the newly developed model configuration including an improved representation of secondary organic aerosol (SOA), i.e., a parametrization for SOA nucleation from natural and anthropogenic precursor gases, have been carried out as intended. The effects of this new SOA scheme have been analysed and evaluated by comparison with aircraft measurement campaigns. A publication describing these developments is currently in preparation. Further improvements to the SOA scheme are in progress, targeting parametrizations depending on highly oxygenated organic molecules (HOMs), the effect of anthropogenic SOA from different emission sectors, and the impacts on clouds and radiation.

5. Model development for the transition from EMAC to ICON and towards GPU capabilities

The development work in view of the future transition to the new base-model ICON, as well as for the use of GPU capabilities, has continued. However, due to the prioritization of other planned work, model simulations with a new ICON-MADE3 configuration have not yet been performed but are planned for the next reporting period. Resources have also been allocated for several short test simulations to ensure binary identity after several technical improvements to the MADE3 aerosol submodel, as part of the ongoing effort in the MESSy consortium to prepare the model for an open-source release.

6. Additional activities

The investigation of the shipping impact on climate under low-sulphur emission scenarios reported in the previous reporting period resulted in the successful completion of the Master Thesis by L. Isselhorst at LMU Munich. During the reporting period, this study was extended by three additional simulations, addressing hypothetical shipping scenarios in which the low-sulphur regulations introduced by the International Maritime Organization in 2020 are applied only in regions with low cloud cover, while retaining high sulphur fuel outside those regions. These additional simulations aimed at investigating the possibility of enhancing the cloud albedo effect while still reducing the air-quality impacts of shipping emissions, in an attempt to solve the climate–air-quality trade-off introduced by these regulations. These results are summarized in a paper recently submitted to Atmos. Chem. Phys. (Isselhorst et al., 2026).

7. Data management

As planned, we have submitted a request to transfer archived data to the long-term archive Doku. This concerns the following dataset groups: DoEfS project (20 datasets, 27.2 TiB); De La Torre Castro et al. (2026) (7 datasets, 2.3 TiB); Isselhorst et al. (2026) (7 datasets, 37.2 TiB). This amounts to a total of 66.7 TiB, closely matching the requested 67 TiB. These resources, however, are not yet allocated, as the request is still being processed by DKRZ data management.