Project: 1499
Project title: ICON-SmART
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Allocation period: 2026-07-01 to 2027-06-30
Co-Principal investigators: Corinna Hoose, Martina Klose, Miriam Sinnhuber

1. Aerosol Developments

We completed our work on coupling of ICON-Seamless with ART aerosol. Specifically, we modified the MEGAN based biogenic emission scheme in ART to incorporate the plant functional types (PFTs) from JSBACH. This required mapping of 11 PFTs from JSBACH to 15 PFTs currently used in ART and followed a similar methodology as reported by Henrot et al. (2017, GMD) with slight modifications to ensure the accurate mapping of PFTs. With this mapping, we have now completed the technical coupling of ICON-Seamless with ART. In addition, we have implemented Anthropogenic emissions for precursor gasses (VOCs, Nitrogen oxides (NOx), Sulfur dioxide (SO_2) Ammonia (NH_3)) and aerosols (BC and OC) in the ICON-ART model from the Emissions Database for Global Atmospheric Research--v8.1 (EDGAR, 2024) dataset. A new subroutine for the online emissions model aerosols has been included by updating the aerosol interface in ART to take into account the anthropogenic aerosol emissions. Furthermore, we have developed a subroutine for the creation of Secondary organic aerosols from precursor gasses – see figure 1.

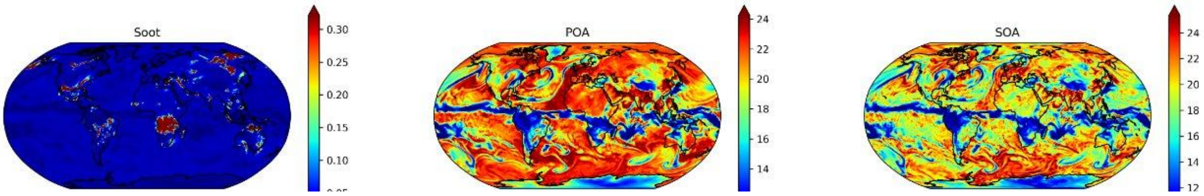

Figure 1: Concentration of soot, primary organic aerosol (POA) and SOA in µg m^{-3} from and ICON-ART simulation

To further our next aim of speeding up ICON-SmART, we have also established a simplified setup by reducing the number of aerosol modes and optimizing the key aerosol dynamical processes – see table. The comprehensive configuration (M4S3) has a total of 45 tracers with 7 aerosol species in 4 modes (Aitken, accumulation, coarse, and giant) and 3 solubility/mixing states (insoluble, soluble, and mixed). While the simplified configurations also have 7 aerosol species, they have different number of tracers depending on the number of modes and mixing states considered. With this simplified aerosol setup, we have achieved a reduction of approximately 27.5% and 30% of computational cost for M2S2-a and M2S2-b, respectively, compared to costs of comprehensive setup We tested these configurations for an extended period of 1 month (January 2020) and a comparison of the global burden of different aerosol species is ongoing.

Aerosol Component	Modes	Solubility
	Comprehensive: M4S3	
Carbonaceous	Accumulation, Coarse	Insoluble/Mixed
Mineral Dust	Accumulation, Coarse, Giant	Insoluble/Mixed
Sea Salt (NaCl)	Accumulation, Coarse, Giant	Soluble/Mixed
Sulfate (SO_4^{2-})	Aitken, Accumulation, Coarse	Soluble/Mixed
Nitrate (NO_3^-)	Aitken, Accumulation, Coarse	Soluble/Mixed
Ammonium (NH_4^+)	Aitken, Accumulation, Coarse	Soluble/Mixed
Water (H_2O)	Aitken, Accumulation, Coarse	Soluble/Mixed
	Simple: M2S3-a and M2S3-b	
Carbonaceous	Accumulation, ~~Coarse~~	Insoluble/Mixed
Mineral Dust	Accumulation, Coarse	Insoluble/Mixed
Sea Salt (NaCl)	Accumulation, Coarse	Soluble/Mixed
Sulfate (SO_4^{2-})	Accumulation, Coarse	Soluble/Mixed
Nitrate (NO_3^-)	Accumulation, ~~Coarse~~	Soluble/Mixed
Ammonium (NH_4^+)	Accumulation, ~~Coarse~~	Soluble/Mixed
Water (H_2O)	Accumulation, ~~Coarse~~	Soluble/Mixed
	Simple: M2S2-a and M2S2-b	
Carbonaceous	Accumulation	Insoluble
Mineral Dust	Accumulation, Coarse	Insoluble
Sea Salt (NaCl)	Accumulation, Coarse	Soluble
Sulfate (SO_4^{2-})	Accumulation, Coarse	Soluble
Nitrate (NO_3^-)	Accumulation, ~~Coarse~~	Soluble
Ammonium (NH_4^+)	Accumulation, ~~Coarse~~	Soluble
Water (H_2O)	Accumulation, ~~Coarse~~	Soluble

Table 1: Aerosol components represented in different model configurations, differing in number of particle size modes (M) and in the number of aerosol solubility states (S).

2. Comprehensive Chemistry

The comprehensive Chemistry portion was mostly completed using the Horeka machine, but has since been transferred to Levante to unify the approach of the assembled ICON-SmART project. We first developed and tested schemes in low resolution (R2B4, ~ 160km). We chose the MOZART-chemistry, in particular the version as described in Sander et al., 2019 (GMD) as our first ansatz for a comprehensive chemistry setup and used the MECCA framework (Sander et al., 2011, 2019,GMD) to implement this mechanism including 247 gas-phase reactions, 65 photolysis reactions for a total of 118 gas-phase species. We performed a 2-month simulation (Jan-Feb 2013) with initialization of 75 tracers and emissions of 7 gases to get an overview of the evolution of all tracers and to study the interplay of emissions and initializations of the trace gases as well as the stability of the chemistry scheme – see figure 2.

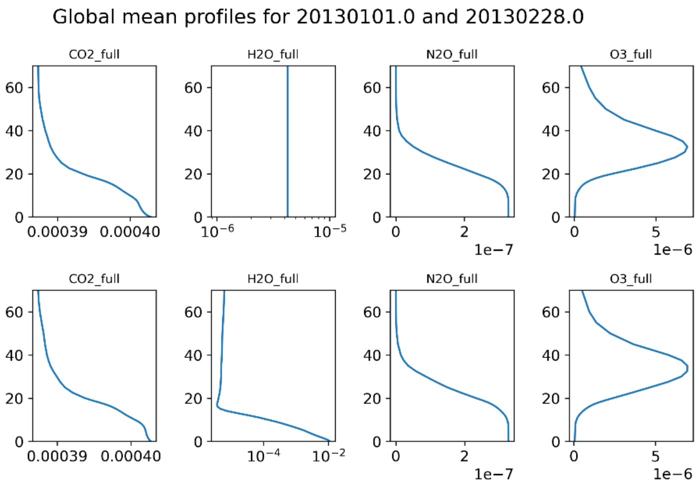

Fig 2: Global mean profiles of the tracers CO_2, H_2O, N_2O, and O_3 at the first time step (initialization, first row) and last time step (second row)

3. Evaluation

In order to evaluate aerosol emission, we built an automated evaluation workflow using auto-icon auto-icon (Baer et al., 2025),a workflow management system that streamlines experimental setup, ensemble generation, configuration handling, and compilation of ICON-SmART. The workflow is now integrating the ESMValTool (Righi et al., 2020, GMD), with auto-icon additionally preparing ICON model outputs, diagnostics, and evaluation scripts in a format compatible with ESMValTool.
We initially applied this workflow to the calibration and evaluation of the dust emission parameterization in ICON-SmART. We conducted multi-member dust tuning experiments over a one-year period, spanning variations in roughness correction, soil-moisture scaling, and land-cover scaling. For evaluation, observations from AERONET (Holben et al. (1998, Remote Sens. Environ.) and the DustCOMM reanalysis (Adebiyi et al. (2020), ACP) were used. For AERONET, a subset of stations following Klose et al. (2021,GMD) was selected, and the workflow filters the observations to retain only "dusty" days using an Ångström exponent–based classifier (AE < 0.3, or as defined by the user) thereby isolating the dust contribution to aerosol optical depth (DOD). The results of the dust tuning experiments are shown in Fig. NUM as a Taylor diagram comparing modelled DOD against observed DOD at AERONET stations. We find an improvement in both correlation and standard deviation from the initial SmART dust emission configuration, which did not include land-cover and soil-moisture scaling, to the subsequent tuning experiments.

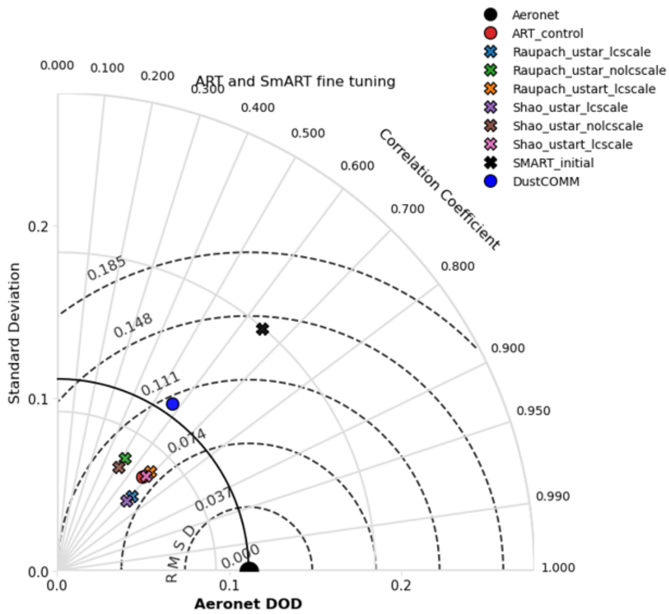

Figure 3: Taylor plot of DOD of various dust tuning experiments against AERONET

Use of resources 07/25-04/26

Regrettably in the past year we have not been able to use our full allocation of resources. The development and testing of the comprehensive chemistry and aerosol setups turned out to be more difficult than expected – and such setups require thorough testing before running the longer benchmark simulations. In particular, the realistic interplay of initialization of chemical tracers, emissions, prescribing of tracers as well as the stability of the numerical scheme has to be assured, also to avoid long spin-up times of the model and wasting high amounts of computation time. We also had to further develop and test our setups and models due to the substantial changes to ICON-ART since it was last tested with the full MECCA chemistry. This resulted in more short test runs, while the longer, computationally very expensive, runs had to be postponed to the end of the reported period and the next phase, respectively.
This, in turn, resulted in much less computation time used than expected in the reported period so far, and a high demand of computation time in the next phase. However, we are confident that we are now in a good position to start the longer benchmark simulations early on in the allocation period, and hence make the most of any resources granted in the next allocation period.