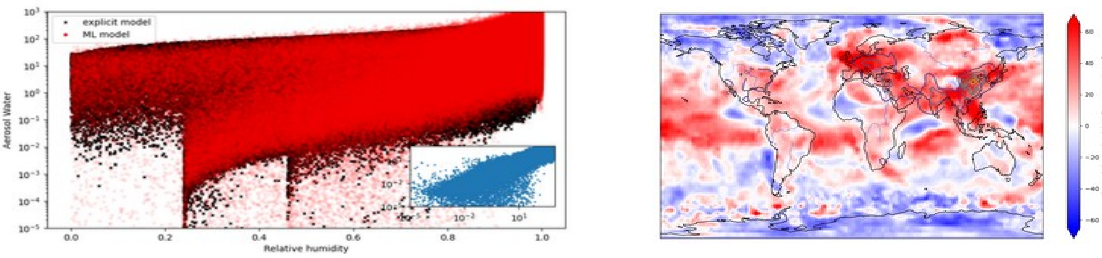
Project: **893**
Project title: **Convection and Clouds in Earth System Modelling**
Principal investigator: **Holger Tost**
Report period: **2022-11-01 to 2023-10-31**
Maximum of 2 pages including figures. 9 pt minimum font size.

In the current allocation period, by far more resources than originally anticipated have been used. This originated from the fact, that in addition to development and maintenance work, as planned one year ago, a substantial set of simulations have been conducted analysing the impact of interactive vegetation calculations on atmospheric chemistry and SOA production.

In the original request for the current allocation period, it was planned to only conduct test simulations for code development. This code development has been dedicated to a new scheme for the optical properties of atmospheric aerosol particles (AOP). For that purpose a new submodel for the EMAC (ECHAM MESSy Atmospheric Chemistry) model in the MESSy (Modular Earth Submodel System) framework has been developed, which can either utilise precalculated lookup-tables as well as online calculations. The same code can be used for both the pre-calculation of the tables as well as online during the simulations, which is a substantial improvement to previous model configurations, in which only two members of the community could perform the required calculations to provide new lookup-tables. Additionally, the new AOP submodel is easily extendable and current developments include the implementation of volcanic ash, as well as brown carbon. Tests are ongoing, and the AOP submodel will be merged into the main devel branch of the MESSy GITLAB project at DKRZ within the current allocation period.
Scientific applications will be conducted in the upcoming allocation period.

A second development part concerned the interactive vegetation, represented in the EMAC system with then help of the LPJ/GUESS model. The coupling had to be intensified and further exchange of variables, especially for deforestation scenarios has been provided. Scientific applications have been conducted in a PhD project (for details, see below).

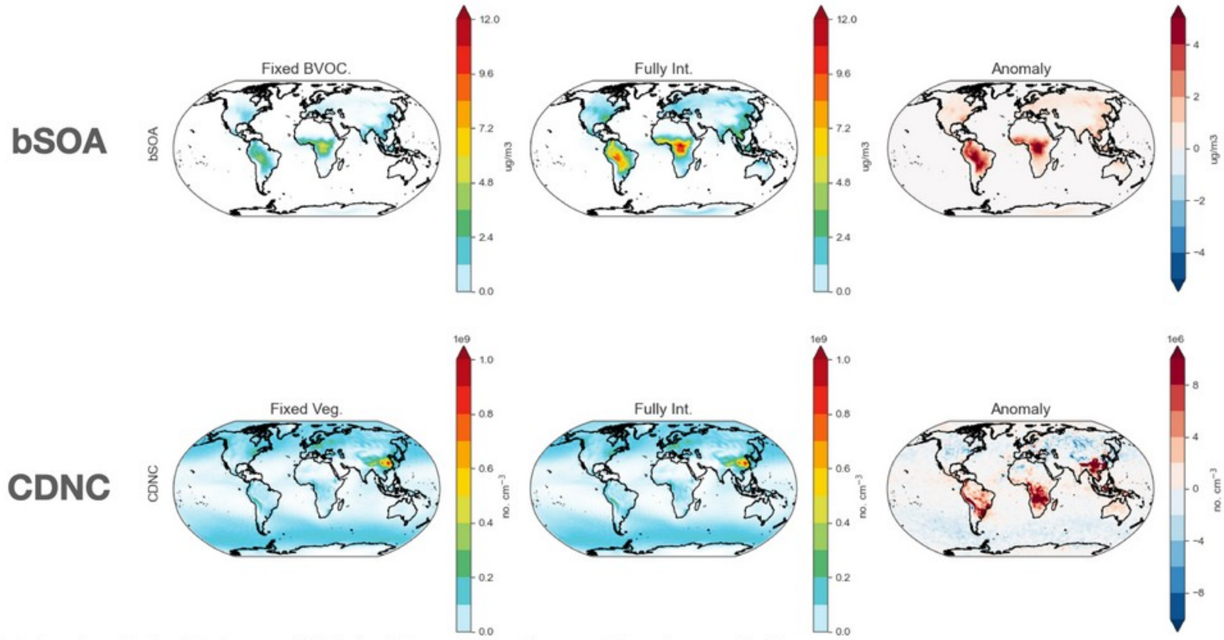
A third development part has been the implementation of the FORTRAN-KERAS-Bridge into the EMAC system. With the help of this infrastructure tool, it is now possible to use pre-trained neural networks (from the KERAS library of Python) online in the FORTRAN code of the EMAC submodel. An application has been the implementation of a neural network of aerosol thermodynamics. Results of this project have been presented at the EGU conference (Vienna, 2023) and a corresponding manuscript is currently in preparation. The Figure 1 indicates, that for e.g., sulphate the neural network provides similar results than the explicit thermodynamics, but with a reduced computational cost.



The left panel shows the calculation of aerosol water in the full parameter space of atmospheric temperatures, and typical aerosol compositions against the relative humidity. The explicit model is depicted by black dots, and the neural network solution by the red data points. The 1:1 correlation (little inserted panel) depicts a relatively good correlation with acceptable deviations. The right panel shows the relative differences in accumulation mode sulphate from the 3D simulation using the neural network compared to the standard explicit thermodynamic calculations with EMAC.

Resulting differences are relatively small, such that the conclusion can be drawn that for climate simulations, where the focus is not on explicit aerosol composition, the neural network implementation provides reasonable results.

In addition to the technical developments, the impact of interactive vegetation on atmospheric chemistry and SOA formation is currently under investigation in a PhD project. As the calculations of atmospheric chemistry, especially with the detailed gas phase mechanism MOM (Mainz organic Mechanism) are quite computationally demanding, a substantial load of CPU hours have been consumed. The study investigates the feedback processes of biogenic emissions from vegetation on aerosol formation and subsequent aerosol radiation and aerosol cloud interactions which lead to modifications of the radiation budget in the atmosphere. The resulting radiative fluxes (direct and diffuse) influence the vegetation growth, expansion and speciation, with resulting implications on biogenic emissions and hence subsequent SOA formation.



Data based on 10 simulated years with full chemistry and interactive vegetation where applicable.
EMAC/LPJ-GUESS models

An example for the biogenic SOA near the surface and the cloud droplet number is provided in Figure 2, where the upper row depicts on the left the biogenic SOA with fixed vegetation against the same quantity with interactive vegetation and hence the above mentioned feedbacks included. The resulting difference is shown in the right panel, stating that there is a substantially more biogenic SOA over the tropical rainforests, if the vegetation can react to the imposed forcing by biogenic aerosol particles. Similarly cloud droplets as depicted in the lower panel of this figure also increase with interactive vegetation leading to potentially more cloud brightening and hence a reduction in near surface radiation.