Project: **893**

Project title: **Convection and Clouds in Earth System Modelling**

Project lead: **Holger Tost**

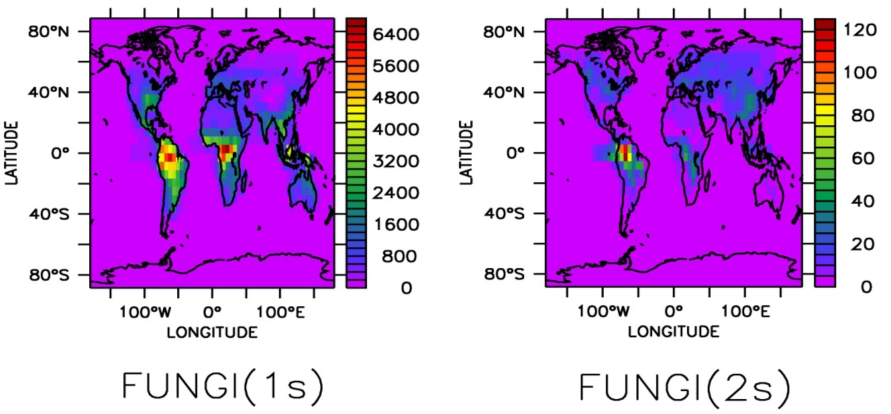
Report period: **2016-01-01 to 2016-12-31**

In the past allocation period only some of the workpackages have been worked on, partly due to the reduction of computational resources and human resources reallocation. Furthermore, a project funding by the DFG has not been successful, such that WPI has not been continued after the end of 2015, WPIII has been refocused (see below), WPIV has been discarded due to staffing shortage, and WPV and WPVI are continuously ongoing.

WPII (PhD project): Global modelling of biological aerosol particles

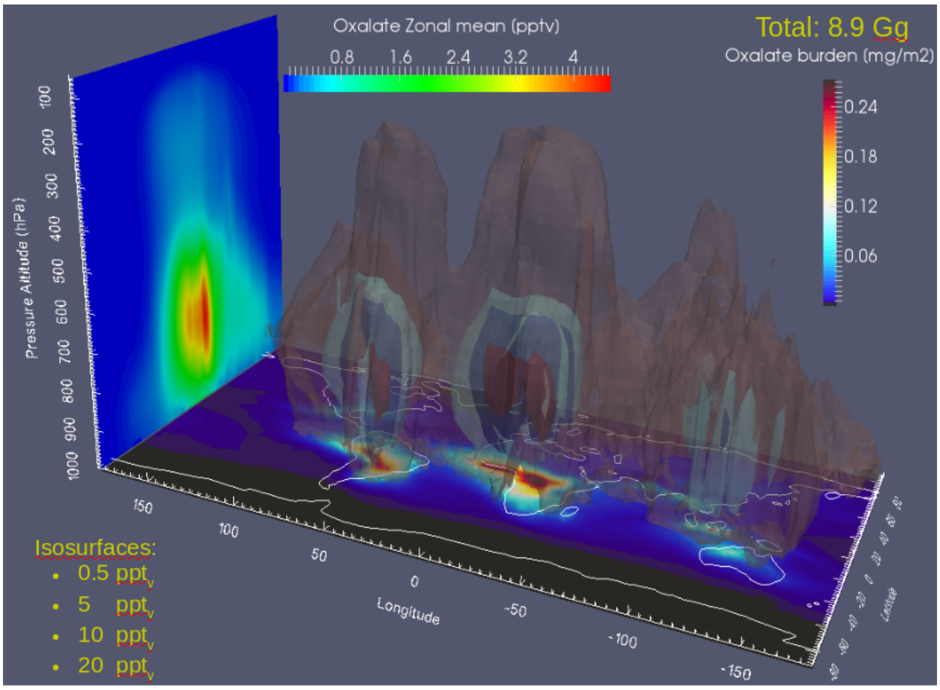
In this WP the PI together with a starting PhD student has performed simulations with passive aerosol tracers to analyse the distribution and deposition of biological aerosol particles with the chemistry-climate model EMAC. Emission functions for bacteria, fungal spores and pollen have been implemented in the model and simulations spanning up to three years have been performed. A comparison with previous studies (Burrows et al., 2009) showed substantial discrepancies, which have been analysed and erroneous results in the latter studies have been confirmed.

In addition to the studies with passive tracers, we have implemented the biological aerosol particles into the dynamical aerosol model GMXE, which included an extension of the lognormal modes to the larger sizes of the bioparticles. Microphysical interactions of the aerosol particles (condensation and coagulation) have been included, which lead to the requirement of corrections in the rediscretisation routine of the lognormal modes, as the old concept proved to be too diffusive. Furthermore, the scavenging scheme for the wet deposition of the bioparticles had to be substantially modified, as the scheme also deals with the re-evaporation of aerosol particles during cloud dissipation and evaporating precipitation. Due to the extended size categories of the aerosol distribution, a new concept for the assignment of the cloud residuals to the aerosol size distribution has been developed. First results are depicted in Fig.1, which shows the mass concentration of fungal spores in the size categories of 0.5 to 1 µm and 1 to 3 µm in 10^{-12} kg/m^3 in the lowest model level. The highest concentrations are found in the tropics close to the emission sources, but also transport over the oceans as well as substantial burdens in high latitudes are found in the simulation results. A significant decrease in the mass concentrations in the larger size categories are simulated due to the modifications in the evaporation and re- discretisation schemes of the EMAC model. Similar results are found for pollen and bacteria. A manuscript on these results is currently in preparation.



WPIII (PI project): Global modelling of oxalates production in clouds

In this WP the cloud processing by aqueous phase chemistry of low molecular weight organic material to oxalates has been investigated. Oxalates are among other species responsible for secondary organic aerosol formation after the evaporation of clouds, which contribute to the background levels of low molecular weight organics worldwide, and have been measured e.g. for the Amazon, but also during the ICCART campaign in the US. To analyse the oxalate formation by clouds the aqueous phase chemistry mechanism of the EMAC model has been extended and simulations have been performed under various assumptions on the cloud processing and the transport within the cloud phase. Fig. 2 shows a 3D visualisation of the global mixing ratios of oxalates (with column burdens in the bottom panel, zonal average distribution at the rear panel and isosurfaces of four levels in the main plot). A substantial amount of oxalates, i.e. almost 9 Gg are produced via the cloud phase. However, this amount is increased more then threefold if transport within the cloud phase is explicitly considered. These findings have gained further importance as also other species such as e.g. formic and acetic acid are simulated with substantially higher burdens compared to the case where cloud processing and transport within the cloud phase have been ignored. The chemical analysis of reaction pathways has shown that oxidation of OH of glycolic acid is the major production pathway of oxalates in clouds. These results have been presented at the ICCP (Internation conference on clouds and precipitation, 2016, Manchester, UK) and a manuscript is currently in preparation.



WPV: Model development and maintenance of the EMAC model

Several test simulations have been performed for the upcoming version of the EMAC modelling system (v 2.53) as well as a few test simulations which have been required to test results of the ESCiMo consortial initiative at DKRZ. Results on this initiative can be found in Jöckel, Tost et al., GMD, 2016).

WPVI: New professorship: Environmental modelling in the climate system

The PI has recently been appointed the new professorship for “Environmental modelling in the climate system” at JGU Mainz. Within this process, he has performed a few test simulations with the MECO(n) system (Mertens et al., 2016), which is a combination of the EMAC model with the COSMO weather forecast model to allow for seamless simulations of atmospheric chemistry and air quality . A few test cases have been calculated with a focus of the Rhein-Main area, but without interactive chemistry.

Literature:

Burrows, S. M., Butler, T., Jöckel, P., Tost, H., Kerkweg, A., Pöschl, U., and Lawrence, M. G.: Bacteria in the global atmosphere – Part 2: Modeling of emissions and transport between different ecosystems, Atmos. Chem. Phys., 9, 9281-9297, doi:10.5194/acp-9-9281-2009, 2009.

Mertens, M., Kerkweg, A., Jöckel, P., Tost, H., and Hofmann, C.: The 1-way on-line coupled model system MECO(n) – Part 4: Chemical evaluation (based on MESSy v2.52), Geosci. Model Dev., 9, 3545-3567, doi:10.5194/gmd-9-3545-2016, 2016.

Jöckel, P., Tost, H., Pozzer, A., Kunze, M., Kirner, O., Brenninkmeijer, C. A. M., Brinkop, S., Cai, D. S., Dyroff, C., Eckstein, J., Frank, F., Garny, H., Gottschaldt, K.-D., Graf, P., Grewe, V., Kerkweg, A., Kern, B., Matthes, S., Mertens, M., Meul, S., Neumaier, M., Nützel, M., Oberländer-Hayn, S., Ruhnke, R., Runde, T., Sander, R., Scharffe, D., and Zahn, A.: Earth System Chemistry integrated Modelling (ESCiMo) with the Modular Earth Submodel System (MESSy) version 2.51, Geosci. Model Dev., 9, 1153-1200, doi:10.5194/gmd-9-1153-2016, 2016.