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*Supplement of*

## **Simulation of the isotopic composition of stratospheric water vapour – Part 1: Description and evaluation of the EMAC model**

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## 1 Introduction

This supplement includes details about the evaluation of the H2OISO submodel within the framework of the EMAC model in the troposphere. For this purpose, the  $^{18}\text{O}$  and D water isotope ratios in precipitation are compared to long-term ground station measurements (GNIP) and to another isotopologue-enabled atmosphere GCM (ECHAM5-wiso).

## 2 Evaluation of EMAC H2OISO in the troposphere

Before applying the EMAC H2OISO submodel in the stratosphere an evaluation of the physical processes in the troposphere was conducted. The representation of the isotope physics in the model can be validated by examining the isotope ratios in precipitation, because these allow to evaluate various isotope fractionation effects (Dansgaard, 1964).

In addition to the EMAC simulation described in the manuscript, another simulation has been carried out for this evaluation. It constitutes a simpler setup (MESSy submodels: H2OISO, CLOUD, CONVECT, CVTRANS, GWAVE, RAD4ALL, TROPOP) without stratospheric chemistry and a resolution of T31L39MA ( $\sim 3.75^\circ \times 3.75^\circ$ , 39 vertical layers, middle atmospheric dynamics). This simulation was performed in “free running” mode, i.e., without Newtonian relaxation to meteorological reference data. The time step of the simulation was twelve minutes and the output is set to produce averaged values for each month. As boundary condition the monthly averages of the climatological sea surface temperatures and sea ice conditions (AMIP11; Hurrell et al., 2008) of the period from 1987 to 2006 were used repeatedly for every year. The last 10 years of a 15 year simulation are used for the evaluation.

### 2.1 Comparison with ground station measurements (GNIP)

Fig. 1 and Fig. 2 show the annual averages of  $\delta^{18}\text{O}(\text{H}_2\text{O})$  and  $\delta\text{D}(\text{H}_2\text{O})$  in precipitation from the two described EMAC simulations, the GNIP database, and the absolute differences between the respective simulation and the GNIP data (see captions). For the lower panels, the annual values of the entire GNIP database were mapped to the respective model grid and subsequently, the absolute value of the difference between the GNIP and the EMAC data was calculated.

Apart from the much lower values of  $\delta\text{D}(\text{H}_2\text{O})$ , compared to  $\delta^{18}\text{O}(\text{H}_2\text{O})$ , which is due to the stronger fractionation in HDO, panels (a) and (b) of Fig. 1 and Fig. 2 show the same patterns. These correspond well between model and measurements (c). On the model grid, only small deviations can be observed between the two model simulations of different resolutions in the respective panels (a) and (b).

The respective panels (d) and (e) reveal large differences in certain regions. The northern regions of Canada and Greenland, the Asian mountains and South Africa show considerable deviations. These can be explained by general discordances in precipitation between model and reality and the poor representation of the model orography. Partly, slight improvements can be seen in the T42L90MA resolution compared to the T31L39MA resolution.

In order to provide an estimate of the representation of the seasonal cycle of  $\delta\text{D}(\text{H}_2\text{O})$  in precipitation between the GNIP measurements and the EMAC model, the monthly averages of the respectively available periods are compared in Fig. 3. For that, particular regions of different climate zones have been defined, chosen to include as many GNIP stations as possible. The defined regions can be seen in the upper left

panel of the figure, which also includes the absolute differences of  $\delta D(H_2O)$  in precipitation from Fig. 2. The regions are labeled with (A) for northern Canada and Greenland, (B) for the Caribbean and parts of Middle and South America, (C) for Patagonia, (D) for Central Europe, (E) for the Middle East, (F) for South Africa and (G) for the eastern parts of China. Additionally to the monthly averages, the standard deviations are included for the two model simulations to provide an estimate of the variation of  $\delta D(H_2O)$ .

In general, the seasonal cycles of the measurements and the simulations correlate well. Some of the regions, however, show large offsets, partly during the entire year, partly in specific seasons. In most cases, the simulation with higher resolution (T42L90MA, green) is closer to the GNIP data, some panels, though, show the opposite. This is due to the different climatic states of both simulations, since the overall temperatures in the T42L90MA simulation are slightly higher than in the T31L39MA simulation and the temperatures determine the strength of the fractionation.

Similar evaluations have been conducted, e.g., by Risi et al. (2010) for the LMDZ-iso model and by Werner et al. (2011) for the ECHAM5-wiso model, albeit, by comparing individual stations instead of regions. These results also feature qualitative good agreement with quantitative comparable deviations in certain climate zones.

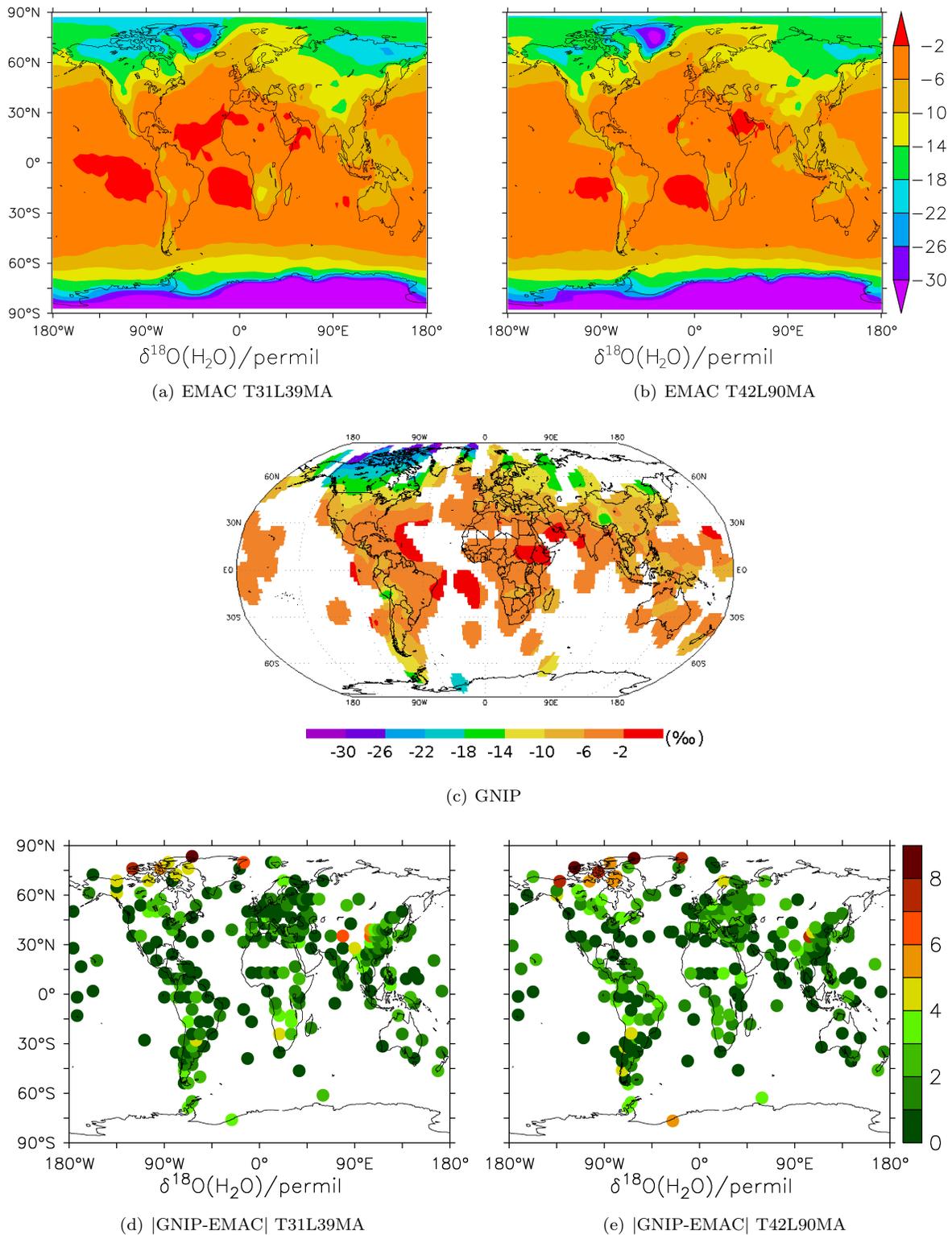


Figure 1:  $\delta^{18}\text{O}(\text{H}_2\text{O})$  in precipitation. EMAC, GNIP and the absolute values of GNIP minus EMAC. EMAC simulations are annual averages of the T31L39MA (a) and the T42L90 (b) simulation. The GNIP data image (c) is taken from IAEA (2001). The absolute differences between GNIP and EMAC are shown for the T31L39MA (d) and for the T42L90MA (e) resolution.

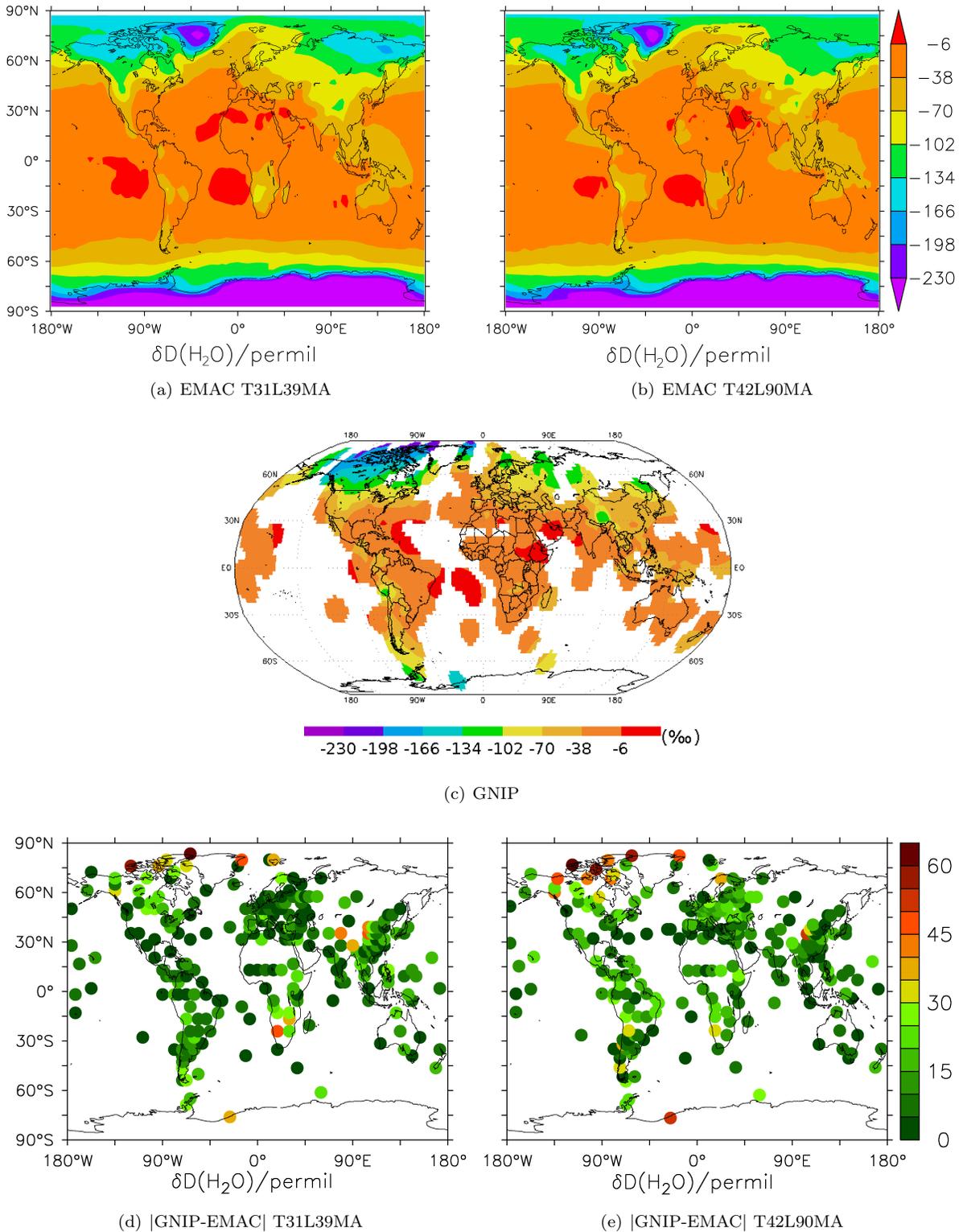


Figure 2:  $\delta D(H_2O)$  in precipitation. EMAC, GNIP and the absolute values of GNIP minus EMAC. EMAC simulations are annual averages of the T31L39MA (a) and the T42L90 (b) simulation. The GNIP data image (c) is taken from IAEA (2001). The absolute differences between GNIP and EMAC are shown for the T31L39MA (d) and for the T42L90MA (e) resolution.

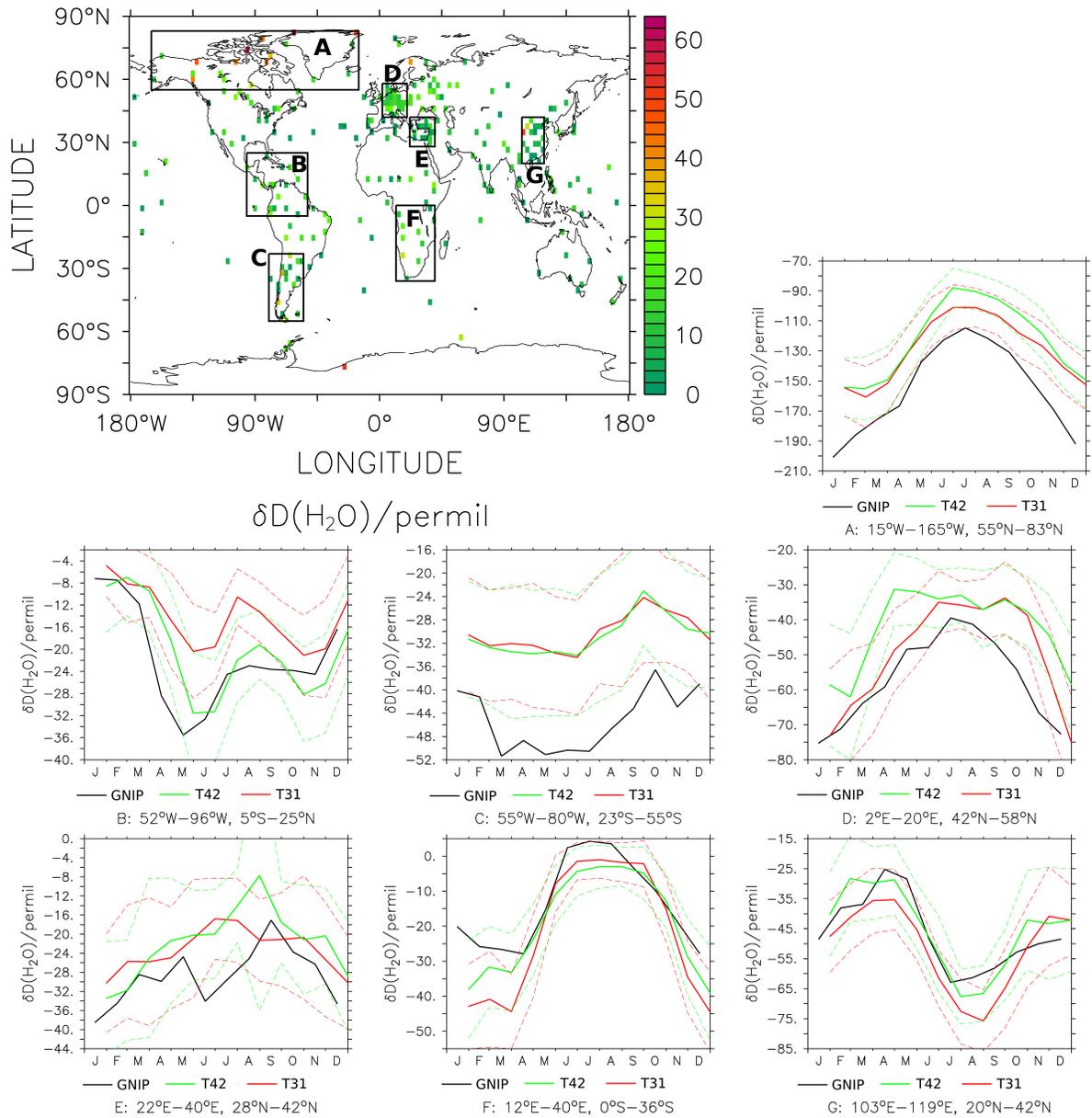


Figure 3: Comparison of the seasonal cycle of  $\delta D(H_2O)$  in precipitation between GNIP data and the two EMAC simulations (T31L39MA and T42L90MA) for selected regions. The map shows the difference between GNIP and EMAC from Fig. 2 and the selected regions (A to G), and the individual panels show monthly averages of the three data sets and the standard deviations (dashed lines) for the two model simulations.

## 2.2 Comparison with ECHAM5-wiso

One of the most recent isotopologue-enabled atmosphere GCMs and the most similar to EMAC is the ECHAM5-wiso model. ECHAM5-wiso has been evaluated successfully against GNIP data in the model resolutions T31L19, T63L31 and T159L31 by Werner et al. (2011). Fig. 4 shows the annual averages of  $\delta^{18}\text{O}(\text{H}_2\text{O})$  in precipitation, globally (top) and for Europe (bottom). The left panels show the T31L39MA and the right panels the T42L90MA resolution. The data is displayed identical to Fig. 1 and Fig. 2 in Werner et al. (2011).

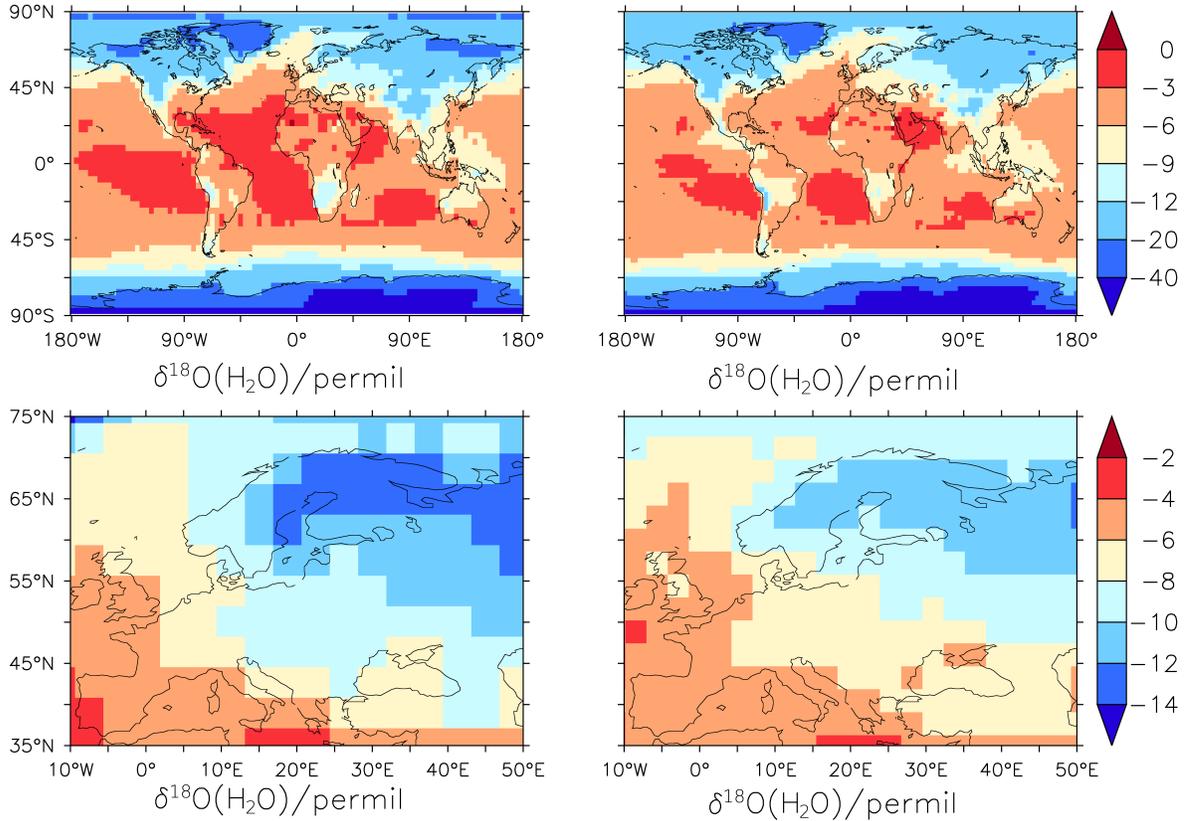


Figure 4: Averaged annual  $\delta^{18}\text{O}(\text{H}_2\text{O})$  in precipitation for the T31L39MA (left panels) and the T42L90MA (right panels) resolution, presented globally (top) and for Europe (bottom).

The patterns and values of the figures agree very well with the ECHAM5-wiso simulations. Especially the ECHAM5-wiso T31L19 simulation shows almost identical results as the T31L39MA simulation of EMAC. The small differences originate mainly from the different boundary conditions, i.e. the sea surface temperatures. The T42L90MA simulation of EMAC fits in, as an intermediate result between the T31L19 and the T63L31 setups of ECHAM5-wiso. The zoom on Europe constitutes only little differences between the two EMAC simulations. The T42L90MA resolution is horizontally still not detailed enough to represent orographic features like the altitude effect in the Alps, which can be observed in the T63L31

and the T159L31 resolution of the ECHAM5-wiso study. The low  $\delta^{18}\text{O}(\text{H}_2\text{O})$  values in Scandinavia and western Russia can not be seen as pronounced anymore in the simulation with higher resolution. This can be explained with the generally warmer conditions in this region in this simulation.

The EMAC simulated averages of  $\delta\text{D}(\text{H}_2\text{O})$  in precipitation in Antarctica (in T42L90MA resolution) are compared with the results from the ECHAM5-wiso model (in T159L31 resolution) from Werner et al. (2011) in Fig. 5. This is conducted, in order to evaluate the fractionation effects at very low temperatures and in the ice phase, which also becomes important when analysing the upper troposphere and the lower stratosphere.

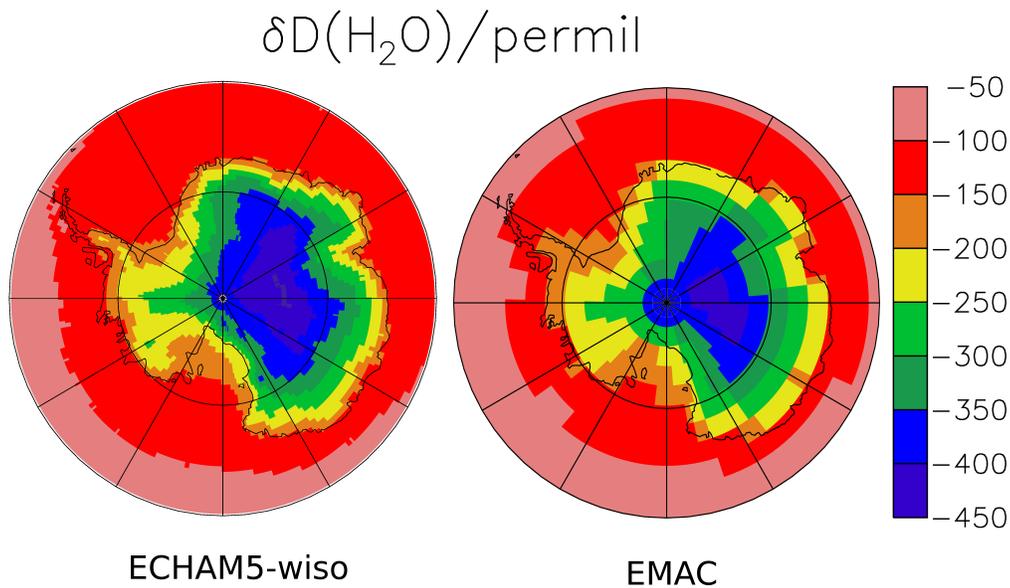


Figure 5: Annual average of  $\delta\text{D}(\text{H}_2\text{O})$  in precipitation in Antarctica from ECHAM5-wiso (in T159L31) (Werner et al., 2011) and EMAC (T42L90MA).

Despite the differences in horizontal resolution, the  $\delta\text{D}(\text{H}_2\text{O})$  in precipitation in Antarctica between the two simulations quantitatively agree very well. The comparison of these results from Werner et al. (2011) with observations compiled by Masson-Delmotte et al. (2008) generally revealed a good agreement. Particular discrepancies can be explained by unresolved effects or general model biases (see Werner et al., 2011).

### 3 Conclusions

The comparison of the EMAC model results with GNIP data generally shows a good agreement, considering the main characteristics, which can be observed in the isotopic composition in precipitation. In most of the regions, also the values, the amplitude and the seasonal cycles compare well with the GNIP measurements. Some regions, though, show considerable differences between model and observations. Since the isotopic composition of precipitation strongly depends on parameters like evaporation and condensation temperatures, the seasonal cycle of the precipitation and also small scale features of the latter, the isotope ratios are very sensitive to the climate conditions. An exact match between model and observations is hence not to be expected. Considering the inaccuracies of the model, but also the difficulties in compiling a representative data set out of partly sparse measurements, the deviations are in a reasonable range.

The results of the simulations of the EMAC model and the ECHAM5-wiso (Werner et al., 2011) model agree very well. Since the hydrological cycles of the two models are basically equal, this was expected. The representation of the isotopologues in the hydrological cycle of the ECHAM5-wiso model technically bases on previous isotopologue-enabled GCMs like ECHAM3 by Hoffmann et al. (1998) and ECHAM4 by Werner et al. (2001). Comprehensive GCM intercomparison studies for stable water isotopologues have been conducted in the SWING (Stable Water Isotope Intercomparison Group) project (Noone, 2006), where also the previous isotopologue-enabled ECHAM versions successfully participated. Hence the conclusion can be drawn, that the EMAC model with the H2OISO submodel represents the state of the art of atmosphere GCMs with explicit representation of the water isotopologues HDO and H<sub>2</sub><sup>18</sup>O in the troposphere.

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