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### 3D distribution of atmospheric vapor isotopes in China, with a focus on tropospheric profiles in monsoon season

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Stable isotopic signals preserved in natural precipitation archives, such as ice cores, provide information on past climatic changes. When measured in the water vapor, water isotopes bear information on large-scale transport, convective and cloud processes.

We present two snapshots of vehicle-based spatially-continuous near-surface water vapor isotopes across a large part of China during the pre-monsoon and monsoon periods. The data documents the spatial and seasonal variability of vapor isotopes and its relationship with large-scale transport and convective activity associated with the monsoon. Seasonal variations in vapor  $\delta$ 180 show the influence of precipitation in the region affected by the summer monsoon, and the influence of temperature in the Northern part. Rayleigh distillation explains spatial variations during the pre-monsoon period, while different moisture source and corresponding atmospheric circulation processes on the pathways are necessary to explain the spatial patterns during the monsoon period. The vapor isotope signals also show that in the pre-monsoon season, the westerlies still controlled the atmospheric circulation in northern China, while the Indian monsoon had already begun in southwest China.

We also made in-situ observation of the vertical profiles of atmosphere vapor isotopes up to the upper troposphere (from the ground surface at 3856m up to 11000m a.s.l.) by implementing specially-designed unmanned-aerial-vehicle system during pre-monsoon, monsoon and post-monsoon periods in the southeastern Tibetan Plateau. We obtained the vertical profiles of vapor isotopes for 77 days totally, including 30 days for which profiles reach 10000m a.s.l or beyond. We aim at better understanding the physical processes controlling the vertical distribution of vapor isotopes, including large-scale transport, microphysical processes, convective mixing and detrainment. We observed the decrease in vapor  $\delta$ 180 that could be attributed to ice detrainment. We observe seasonal and intra-seasonal variations that are vertically coherent, with more depleted values during the monsoon season and in October.

### A fully coupled isotope-enabled Earth system model ensemble dataset under historical and future forcing

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Water isotope ratios are an integrated signal of how water moves through the atmosphere, from evaporation, through transport and phase changes, to its final point of precipitation. Isotopeenabled Earth system models allow for the direct simulation of water isotopologues within the Earth system, and are a valuable tool for improving our understanding of the past and present global water cycle. However, to date, isotope-enabled simulations have been primarily used to study past climates, or employed in atmosphere-only or low complexity models. Understanding how water isotope ratios will respond in future climates within a fully coupled system could give critical insight into how the global water cycle is changing. Here, we present a new ensemble dataset from the fully coupled isotope-enabled version of the Community Earth System Model version 1.2 (iCESM1.2), run with historical and RCP8.5 forcing. The dataset includes outputs of water isotope ratios in the atmosphere, land, and ocean. We also trace the movement of water through the atmosphere using numerical water tracers, a direct measure connecting evaporative sources to precipitation sinks. Combining isotope ratios with numerical water tracers will build a better understanding of how relationships between evaporative sources, moisture transport, and isotope ratios are expected to manifest in the real world. Additionally, isotope ratios may provide a more coherent signal than more conventional metrics like precipitation, thereby enabling earlier detection of atmospheric water cycle change. We present our model configuration, available outputs, and preliminary results. Our early findings suggest that large-scale changes in atmospheric water isotope ratios occur as the world warms, and that these changes are consistent with expected changes in moisture transport. This dataset will help us better understand the dynamics of the shifting global water cycle under present-day climate change. Our aim is to make this dataset available to the general scientific community to aid future water isotope research and further our understanding of how the global water cycle is projected to change.

### A new theoretical framework for parameterizing nonequilibrium fractionation during evaporation from the ocean

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The evaporation isotope model proposed by Craig and Gordon (1965) is used in most atmospheric isotope models for the parameterization of fractionation during evaporation from the ocean. It describes the isotope ratios in the evaporation flux as a function of the isotope ratios in liquid water and the atmosphere, relative humidity, the equilibrium fractionation factor, and the nonequilibrium fractionation factor (k iso). Of these parameters, k iso is the most uncertain. Many isotope models use the formulation of Merlivat and Jouzel (1979), which parameterizes k iso as a function of wind speed and distinguishes between a smooth and a rough regime to account for the fact that waves act as roughness elements, inducing perturbations that significantly influence gas transfer rates. The resulting discontinuity in k iso and therefore isotope ratios, which usually occurs at around 7m/s wind speed, has been disputed by several empirical studies, based on measurements of deuterium excess and 17O-excess in the near-surface boundary layer (e.g., Pfahl and Wernli, 2009; Uemura et al., 2010; Bonne et al., 2019). However, a theoretical framework, which would be in line with the measurements, is still lacking. Here, we present a new approach to parameterizing k iso by explicitly accounting for the influence of wave drag on the momentum flux near the surface. Following recent work by Cifuentes-Lorenzen et al. (2018), we add a third wave-induced component to the total momentum flux, in addition to the viscous and turbulent components, and extend the definition of the eddy viscosity to account for the loss of friction velocity due to waves and the fall-off of turbulence close to the surface. The new scheme predicts a slight decrease of k iso with wind speed, similar to the values from Merlivat and Jouzel (1979) if the smooth-regime parameterization were used at all wind speeds. This new parameterization will be incorporated into the isotope-enabled Community Earth System Model to test its fidelity.

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#### Abrupt Heinrich Stadial 1 cooling missing in Greenland oxygen isotopes

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Abrupt climate changes during the last deglaciation have been well preserved in proxy records across the globe. However, one long-standing puzzle is the apparent absence of the onset of the Heinrich Stadial 1 (HS1) cold event around 18 ka in Greenland ice core oxygen isotope  $\delta$ 180 records, inconsistent with other proxies. Here, combining proxy records with an isotope-enabled transient deglacial simulation, we propose that a substantial HS1 cooling onset did indeed occur over the Arctic in winter. However, this cooling signal in the depleted oxygen isotopic composition is completely compensated by the enrichment because of the loss of winter precipitation in response to sea ice expansion associated with AMOC slowdown during extreme glacial climate. In contrast, the Arctic summer warmed during HS1 and YD because of increased insolation and greenhouse gases, consistent with snowline reconstructions. Our work suggests that Greenland  $\delta$ 180 may substantially underestimate temperature variability during cold glacial conditions.

#### Advances in water isotope observation, simulation, and model-data integration

#### Kei Yoshimura, Institute of Industrial Science, The University of Tokyo

In the last two decades, hydro-meteorological studies using water isotope ratios have changed dramatically on a global scale. In particular, two technological innovations have contributed greatly to this change. One is the development of water isotope ratio observation technology using spectroscopic analysis, and the other is the development of water isotope models, such as the water isotope general circulation models. Recently, the author's group has been conducting water isotope ratio data assimilation studies using both the technological advances, as an example of model-data integration.

In this talk, I introduce an experimental study of idealized data assimilation using the observed distribution of water isotope ratios by satellite initiated by Yoshimura et al. (2014), and some recent achievements by Toride et al. (2021) for more detailed analysis on why the isotope could improve the atmospheric circulation fields and Tada et al. (2021) for a study of data assimilation of actual satellite observations.

Water vapor isotope ratios observed by the IASI spectroscopic sensor onboard the European MetOp satellite were assimilated with the results of simulations by the IsoGSM global isotope atmospheric general circulation model to estimate water vapor isotope ratio distributions more accurately and to determine how much the atmospheric environmental elds such as wind speed, air temperature, and specific humidity are improved by the data assimilation. Although the number of water isotope observations by IASI is about one fiftieth of the number of existing operational observations, it was confirmed that the wind speed, specific humidity, and temperature elds in the middle troposphere improved by more than 10% in ideal experiments when additional water isotope ratios were assimilated. The impact on the thermodynamic structure of the tropics is then analyzed, and it is shown that the effect of water isotope ratio observations is dominant in the upwelling part of the Hadley circulation, where convective activity is high, and results in non-local improvements throughout the large- scale circulation. Furthermore, by applying the variable localization method of data assimilation, we elucidated that the thermodynamic process (phase change) is more important for improving the accuracy of prediction than the dynamical process (transport) of isotope ratios.

Based on the above, we conducted an actual data assimilation experiment of IASI from April 1 to April 30, 2013, in which only the observed water isotope ratios of IASI were data- assimilated, and a no-observation experiment in which no data was assimilated. During the data assimilation period, the data assimilation of the actual observed water isotope ratios improved the accuracy of the analysis of many meteorological variables including temperature as well as water isotope ratios. As an example, according to the time series of errors between the experiment with assimilated IASI isotope ratios and the no-observation experiment, it is clearly shown that the IASI assimilation experiment is more accurate than the no-observation experiment not only for the water vapor isotope ratio  $\delta$ 2H in the middle troposphere, but also for the surface air temperature.

#### Water Isotope Enabled Modeling: recent progress & next steps

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Climate models are widely employed to assess our physical understanding of Earth, examine robust features of future climate change projections, and test hypotheses surrounding large-scale climate phenomena. Given their powerful ability to capture both hydroclimate and circulation processes, from moisture source and history of convection to local temperature, water isotopes are now commonly-added tracers in GCMs, and have been incorporated into the atmosphere, ocean, and land surface components of models. Water isotopes provide key constraints on model simulations of the hydrological cycle, and can yield unique insights surrounding current parameterizations of mixing or large-scale circulation, for example.

This overview talk will provide a historical perspective on water isotope enabled modeling efforts across time (paleoclimate and modern) and across spatial scales (e.g. Large-Eddy Simulations vs. GCMs). The US CLIVAR Water Isotope Working Group developed several key areas for scientific inquiry that water isotope-enabled modeling efforts can uniquely address in future work. Furthermore, the increasing availability of water isotope retrievals from remote sensing products (e.g. TES, AIRS) and in-situ water vapor isotope measurements facilitate novel comparisons against water isotope observations, which can provide key constraints on Earth system processes and model physics. A review of key opportunities and challenges forthcoming in the realm of isotope-enabled model simulations and experiments will be discussed.

Importantly, both the Coupled Model Intercomparison Project (CMIP) and the Paleoclimate Model Intercomparison Project (PMIP) have successfully provided common experiments and boundary conditions, applied equally across multiple simulations, to test for differences between models and coherent responses to external forcing. To-date, however, such MIP efforts have not included critical variables for comparison in their history files: water isotopes. While a large number of efforts have been made to incorporate water isotope physics and tracers into atmospheric general circulation models, large-scale intercomparisons across modeling groups focused on water isotope fields have not been performed since 2012 (SWING2, Risi et al., 2012; https:// data.giss.nasa.gov/swing2/). The Stable Water Isotope Intercomparison Group (SWING) is ready for round 3! Such comparisons are sorely needed to advance our understanding of how Earth's climate will respond to pervasive anthropogenic forcing.

Thus, this presentation will duly serve as a call to action for isotope-enabled modelers to come together internationally and perform the next round of isotope enabled inter-model simulations and comparisons. We hope to discuss and solicit feedback on a formal set of scientific goals, working hypotheses, experimental designs and model simulations for SWING3 throughout the course of the workshop.

#### Analytical procedures for water isotope analysis at FARLAB

#### Pål Tore Mørkved, Department of Earth Science, University of Bergen Harald Sodemann, Geophysical Institute, University of Bergen

The Facility for Advanced Isotopic Research and Monitoring of Weather, Climate and Biogeochemical Cycling (FARLAB) at University of Bergen, provides as part of their analytical portfolio services for the measurement of the stable isotopes in liquid water and water vapour. The analysis, post-processing, and calibration of the raw analytical signal onto the VSMOW-SLAP reference scale includes a number of critical procedures to counteract instrumental drift, intersample memory effects, and the correct quantification of total uncertainty. Here we present the currently used analytical procedures for both saline and freshwater liquid samples with regard to  $\delta D$ ,  $\delta 180$ , and  $\delta 170$ , and the post-processing and calibration using the software routines FLIIMP developed at FARLAB. Furthermore, we present the post-processing and calibration procedures for ambient vapour measurements, using the software routines FaVaCal developed at FARLAB. Inter-comparison of such procedures with other stable isotope laboratories is central in providing well-documented, high-quality data with fully quantified and small uncertainty to the community.

#### Are empirical equations able to calculate stable isotopes content of vapor correctly?

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The stable isotopes in precipitation can present valuable information regarding the hydrological cycle (Clark and Fritz, 1997). Furthermore, stable isotopes in the vapor can also present precious information which helps to understand meteorological processes as well as the climatic system functions accurately. The stable isotopes in a water molecule are affected by three main processes such as the equilibrium isotopic fractionation between water and vapor, kinetic evaporation (which is strongly dependent on the air humidity (h)), and the mixing process (Clark and Fritz, 1997). The stable isotopes content in the vapor can be directly measured or calculated by empirical equations using the stable isotopes content of precipitation. In this study, the comparison between the calculated and measured stable isotopes content of vapor has been conducted by the isotope content in the vapor was calculated from the precipitations using equations 1 to 4 (Clark and Fritz, 1997).

| $\Delta \epsilon = 180$ water-vapor = -14.2 (1-h) ‰                           | (1) |
|-------------------------------------------------------------------------------|-----|
| $\Delta \epsilon = 2H$ water-vapor = -12.5 (1-h) ‰                            | (2) |
| $\delta$ 18O water - $\delta$ 18O vapor = ε18O water-vapor +Δε18O water-vapor | (3) |
| $\delta$ 2Hwater - $\delta$ 2H vapor = ε2H water-vapor + Δε2H water-vapor     | (4) |

The equilibrium isotopic fractionations between water and vapor ( $\epsilon$ ) at 25 °C are about -9.3 ‰ and -76 ‰ for 18O and 2H, respectively (Clark and Fritz, 1997). The isotopic fractionation in the kinetic conditions of evaporation has been determined using equations 1 and 2 for 18O and 2H, respectively. The total fractionation between water and vapor was calculated using equations 3 and 4 for 18O and 2H isotopes, respectively.

Due to the effect of significant evapotranspiration in a rice paddy, the measured and calculated isotopes value in the vapor were not completely matched. The results demonstrated that the dominant differences between the measured and calculated isotope values mainly for  $\delta$ 180 occurred during the hot months June, July, and August when the temperature and evaporation showed the highest values. However, during the cold months (December to February) when temperature and evaporation decreased dominantly, the role of evaporation significantly declined on stable isotopes content of vapor. Therefore, the measured and calculated isotopes in vapor showed approximately the same contents.

The results of this study show that stable isotopes content of vapor can be calculated using the empirical equations using the stable isotopes content of precipitation with high accuracy in the regions where the evaporation is not significant and minimal. However, in the regions with high evaporation, empirical equations can't calculate stable isotopes content of vapor accurately.

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### Atmospheric water vapour isotopes in the Arctic at the interface with sea ice and open ocean

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Due to the recent and severe downtrend in sea ice coverage, Arctic-derived moisture serves as new, increasingly important, water source for the northern hemisphere. Feedback and exchange processes between the different hydrological compartments of the Arctic might be tracked by stable water isotopologues (H216O, H218O, HD16O). This is possible as evaporative sources, phase changes and transport history have a specific imprint on the isotopic compositions. The MOSAiC drift experiment offered the unique possibility to tackle the main hydrological processes occurring in the Central Arctic, covering a complete seasonal cycle, including the understudied Arctic winter. A Cavity Ring Down Spectrometer (CRDS) was installed on board of RV Polarstern and atmospheric humidity,  $\delta$ 18O,  $\delta$ D and d-excess were observed continuously from October 2019 to October 2020. Simultaneously, isotopic changes of water vapour have been measured by international partners at several land-based Arctic stations.

A first analysis of the Polarstern isotopic vapour dataset reveals a range of 30‰ (min=-48.4; max=-11.4; mean=-32.4) variations in  $\delta$ 180 of atmospheric water vapour. A clear seasonal cycle with the most depleted values occurring in the dry and cold winter months and increasingly enriched values in spring, peaking in August is noticed. Strong, positive correlation is found with both local specific humidity (r2 = 0.87) and air temperature (r2=0.81). Several short-term events on synoptical time scales with abrupt fluctuations in the isotopic composition are detected throughout the entire dataset, especially during the freeze up phase (Oct-Nov) and the transition from frozen conditions to summer melt (Apr-Jun). Preliminary comparison of the Polarstern data with measurements from different Arctic stations indicates a strong influence of sea ice coverage on the isotopic signal.

For an in-depth understanding of the observed isotopic changes, we quantitatively compare the measured isotopic signatures with model results from an ECHAM6 atmosphere simulation, which includes explicit water isotope diagnostics. For this simulation, pressure and temperature fields have been nudged to ERA5 data. The model-data comparison assesses the capability of this state-of-the-art AGCM to capture the first-order evaporation/condensation processes and their seasonal evolution. However, both a systematic overestimation of winter values and overall decreased variability of modeled isotope values as compared to the observation is found. Investigation of such discrepancies may help to identify deficits in the representation of the fine-scale exchange processes characterizing the central-Arctic water cycle.

# Can the assimilation of IASI water isotopolologue observations improve the quality of tropical diabatic heating?

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The strong coupling between atmospheric circulation, moisture pathways and atmospheric diabatic heating is responsible for most climate feedback mechanisms and controls the evolution of severe weather events. However, diabatic heating rates obtained from current meteorological reanalysis show significant inconsistencies. Here, we theoretically assess with an Observation System Simulation Experiment (OSSE) the potential of the MUlti-platform remote Sensing of Isotopologues for investigating the Cycle of Atmospheric water (MUSICA) Infrared Atmospheric Sounding interferometer (IASI) mid-tropospheric water isotopologue data for constraining uncertainties in meteorological analysis fields. We use the Isotope-incorporated General Spectral Model (IsoGSM) together with a Local Ensemble Transform Kalman Filter (LETKF) and assimilate synthetic MUSICA IASI isotopologue observations. We perform two experiments consisting each of two ensemble simulation runs. In the first experiment, we perform a simulation run where observations (temperature, humidity and wind profiles obtained from radiosonde and satellite data) are assimilated and compare this to a simulation run where additionally to the conventional observations the synthetic IASI isotopologue data are assimilated. In the second experiment, we perform a simulation run where only synthetic IASI isotopologue data are assimilated and another one where no observational data at all are assimilated. The first experiment serves to assess the impact of the IASI isotopologue data additional to the conventional observations and the second one to assess the direct impact of the IASI isotopologue data on the meteorological variables, especially on the heating rates and vertical velocity. The assessment is performed for the tropics in the latitude range from 10°S to 10°N. When the synthetic isotopologue data are additionally assimilated, we derive in both experiments lower Root-Mean-Square Deviations (RMSDs) and improved skills for precipitation and all other meteorological variables (improvement by about 8-13%). However, heating rates and vertical motion can only be improved throughout the troposphere when additionally to IASI  $\delta D$  conventional observations are assimilated. When only IASI  $\delta D$  is assimilated the improvement in vertical velocity and heating rate is minor (up to a few percent) and restricted to the mid-troposphere. These results nevertheless reveal the potential of the temporally and spatially highly resolved isotopologue data from IASI to reduce the uncertainties of diabatic heating rates in the tropical regions and therefore not only improving the meteorological analyses but in consequence also weather forecasts and climate predictions.

# Cloud microphysical processes and stable water isotopes during ISLAS 2020 campaign in Svalbard

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Physical processes in Arctic clouds are not well represented in the numerical weather prediction and climate models. Composition of stable water isotopes in precipitation and vapour can be used to track phase changes during cloud formation, within and below the clouds and improve our understanding of these sub-grid scale transformations.

We performed water vapour and precipitation measurements during spring ISLAS 2020 campaign in Ny-Ålesund, Svalbard, to study the isotopic signal of cold-air outbreaks (CAOs) and warm air intrusions (WAIs). The thermodynamic conditions during several CAO and WAI regimes were studied using ground-based measurements, Cloudnet and radiosonde profiles.

The isotopic composition of the equilibrium vapour from the precipitation samples showed strong correlation with the vapour measured at the Zeppelin station at 474 m a.s.l. Snow was more depleted in heavy isotopes than surface vapour, indicating that a large portion was formed aloft at colder temperatures.

During the CAOs, local ice nucleation events and shallow stratiform clouds were observed. The ice particles formed via vapour deposition on the ice nuclei, and additional riming was detected when supercooled droplets were present on the top of the atmospheric boundary layer (ABL). The elevated d-excess values were detected in vapor measurements indicating strong kinetic fractionation due to evaporation in unsaturated conditions. In the presence of precipitating single low-level clouds, similar isotopic signatures were detected in the snow samples as well. During the WAIs, the temperature and cloud top height increased, and a thin layer of cloud droplets was identified on the top of the supercooled droplets and ice clouds. Despite presence of multi-layer clouds, the isotopic signal, characterized by increased  $\delta 180$ ,  $\delta$  D and d-excess values, was similar in vapour and precipitation due to enhanced mixing creating uniform specific humidity profiles and facilitating spontaneous riming of supercooled droplets on the ice particles in the lower cloud level.

The discrepancy between the precipitation and vapour data was observed during the presence of clouds and specific humidity inversions above the ABL. Both features indicate the importance of considering contribution from different vapour sources during snow formation for interpretation of precipitation samples.

# Continuous monitoring of surface water vapour isotopic compositions at Neumayer Station III, East Antarctica

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In this study, the first fully-continuous monitoring of water vapour isotopic composition at Neumayer Station III, Antarctica, during the two-year period from February 2017 to January 2019 is presented. Seasonal and synoptic-scale variations of both stable water isotopes H218O and HDO are reported, and their link to variations of key meteorological variables are analysed. Changes in local temperature and humidity are the main drivers for the variability of  $\delta$ O18 and  $\delta$ D in vapour at Neumayer Station III, both on seasonal and shorter time scales. In contrast to the measured  $\delta$ O18 and  $\delta$ D variations, no seasonal cycle in the Deuterium excess signal d-excess in vapour is detected. However, a rather high uncertainty of measured d-excess values especially in austral winter limits the confidence of this finding. Overall, the d-excess signal shows a stronger inverse correlation with humidity than with temperature, and this inverse correlation between dexcess and humidity is stronger for the cloudy-sky conditions than for clear-sky conditions during summertime. Back trajectory simulations performed with the FLEXPART model show that seasonal and synoptic variations of  $\delta$ O18 and  $\delta$ D in vapour coincide with changes in the main sources of water vapour transported to Neumayer Station. In general, moisture transport pathways from the east lead to higher temperatures and more enriched  $\delta O18$  values in vapour, while weather situations with southerly winds lead to lower temperatures and more depleted  $\delta O18$ values. However, for several occasions,  $\delta O18$  variations linked to wind direction changes were observed, which were not accompanied by a corresponding temperature change. Comparing isotopic compositions of water vapour at Neumayer Station III and snow samples taken in the vicinity of the station reveals almost identical slopes, both for the  $\delta O18-\delta D$  relation and for the temperature– $\delta$ O18 relation.

# Contribution of the Southern Annular Mode to variations in water isotopes of daily precipitation at Dome Fuji, East Antarctica: A study with an isotope-enabled AGCM MIROC5-iso

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Water isotopes measured in Antarctic ice cores enable reconstruction at the first order of the past temperature variations. However, the seasonality of the precipitation and episodic events, including synoptic-scale disturbances [1,2], influence the isotopic signals recorded in ice cores. We used a Japanese isotope-enabled atmospheric general circulation model AGCM, MIROC5-iso [3], to investigate variations in climatic factors in  $\delta$ 180 of precipitation ( $\delta$ 180p) at Dome Fuji, East Antarctica. A simulation was conducted with the horizontal winds nudged to the JRA-25 reanalysis [4] from 1981 to 2010 and nicely reproduced the observed daily  $\delta$ 180p at Dome Fuji in 2003 [1], as well as the related synoptic precipitation events. We revealed that the Southern Annular Mode (SAM), the primary mode of atmospheric circulation in the southern mid-high latitudes, significantly contributed to the daily isotope signals at Dome Fuji. Positive  $\delta$ 180p anomalies, especially in the austral winter, were linked to the negative polarity of the SAM (SAM-), which weakens westerly winds and increases the southward inflow of water vapor flux. SAM-contributed to the precipitation of heavy  $\delta$ 180p at Dome Fuji as a locational feature and less contributes at Dome C. A revised manuscript of this study is under review in J. Geophys. Res. Atmos. (https://doi.org/10.1002/essoar.10507344.3).

### Data assimilation using oxygen isotope ratios of proxies aimed at the last millennium climate reconstruction

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Data assimilation combines both proxies and climate models, and can reconstruct the past climate change. We use the offline data assimilation approach which regards annual values of a single simulation as an ensemble member, and assimilates the ensemble mean with values of proxies. This study has so far tried to reconstruct the annual variations of climatic variables over the last millennium by assimilating oxygen isotope ratios of corals, ice cores, and tree rings. In addition, new experiments using speleothem data (Comas-Bru et al., 2020) and the proxy model of speleothem are conducted. By incorporating these speleothem records and, the amount of proxies that can be used in this study increases from 129 to 257.

We compared the annual variations of surface air temperature in the experiment with and without speleothem data. In the experiment with speleothem data, temperature decline in Asian region after the volcanic eruption in 1257 can be represented whereas it cannot be represented in the experiment without speleothem data. This difference between the two experiments shows the influence of using speleothem data because there are few proxies available in Asian region before using speleothem data in the 13th century. On the other hand, there is no large difference in the reconstructed annual surface air temperature variations between the two experiments in the 20th century although the number of available proxies is increased. We conducted pseudoproxy experiments in the 20th century. The results suggest that the relationship between the number of proxies and the impact of proxies on the reconstructed variations is close to a linear relationship. It is suggested that there are sufficient proxies to reproduce the variations in 20th century, and that adding speleothem data makes no large difference.

# Deep Learning for Estimating High Temporal Resolutions of Stable Water Isotope Concentrations

#### Thomas Y. Chen (Academy for Mathematics, Science, and Engineering)

Recent advances in laser spectroscopy has made it feasible to measure stable isotopes of water in high temporal resolution (i.e., sub-daily). High-resolution data allow the identification of finescale, short-term transport and mixing processes that are not detectable at coarser resolutions. Despite such advantages, operational routine and long-term sampling of stream and groundwater sources in high temporal resolution is still far from being common. Methods that can be used to interpolate infrequently measured data at multiple sampling sites would be an important step forward. This study investigates the application of a Long Short-Term Memory (LSTM) deep learning model to predict complex and non-linear high-resolution (3 h) isotope concentrations of multiple stream and groundwater sources under different landuse and hillslope positions in the Schwingbach Environmental Observatory (SEO), Germany. The main objective of this study is to explore the prediction performance of an LSTM that is trained on multiple sites, with a set of explanatory data that are more straightforward and less expensive to measure compared to the stable isotopes of water. The explanatory data consist of meteorological data, catchment wetness conditions, and natural tracers (i.e., water temperature, pH and electrical conductivity). We analyse the model's sensitivity to different input data and sequence lengths. To ensure an efficient model performance, a Bayesian optimization approach is employed to optimize the hyperparameters of the LSTM. Our main finding is that the LSTM allows for predicting stable isotopes of stream and groundwater by using only short-term sequence (6 h) of measured water temperature, pH and electrical conductivity. The best performing LSTM achieved, on average of all sampling sites, an RMSE of 0.7%, MAE of 0.4%, R2 of 0.9 and NSE of 0.7. The LSTM can be utilized to predict and interpolate the continuous isotope concentration time series either for data gap filling or in case where no continuous data acquisition is feasible. This is very valuable in practice because measurements of these tracers are still much cheaper than stable isotopes of water and can be continuously conducted with relatively minor maintenance.

#### Density of recent isotope observations in the European storm track region

#### Harald Sodemann, Geophysical Institute, University of Bergen, Norway

The water cycle in atmospheric and coupled models is a major contributor to model uncertainty, in particular at high-latitudes, where contrasts between ice-covered regions and the open ocean fuel intense heat fluxes. However, observed atmospheric vapour concentrations do not allow us to disentangle the contributions of different processes, such as evaporation, mixing, and cloud microphysics, to the overall moisture budget. As a natural tracer, stable water isotopes provide access to the moisture sources and phase change history of atmospheric water vapour and precipitation. This work compiles currently available observations of the isotope composition in water vapour, precipitation, ocean, and land surface waters in the European storm track region. Wide spatial coverage, multi-platform measurements, and inclusion both of water vapour and precipitation make this region particularly well-suited for future data-model comparison studies with isotope-enabled models. In addition to enabling improved isotope-enabled models from observations along the entire water transport history, I emphasize the potential for improving our understanding of water cycle processes and the role of diabatic processes in the storm track on different time scales, from weather to climate to paleoclimate.

#### Detecting precipitation vs. mixing in shallow cloud marine boundary layers

#### Dean Henze, College of Earth, Ocean and Atmospheric Sciences, Oregon State University David Noone, Department of Physics, Waipapa Taumata Rau (The University of Auckland)

Climate models show large variability in stratocumulus-topped marine boundary layer (StCMBL) cloud representation. The formation of stratocumulus clouds is linked to the energy and moisture budgets of the marine boundary layer and there is a need for tighter observational constraints on these budgets. Because coupled measurements of water vapor and its stable heavy isotope ratios can distinguish between precipitation and simple airmass mixing, for example on  $q-\delta D$ diagrams, they have the potential to tighten moisture budget constraints not easy to obtain with traditional thermodynamic variables. While vertical profiles of isotope ratios through the marine boundary layer are sparse, recent observational campaigns such as ORACLES (ObseRvations of Aerosols above CLouds and their intEractionS) provide the data to start addressing such research guestions. This study uses data from the ORACLES campaign collected with the Water Isotope System for Precipitation and Entrainment Research (WISPER) to assess q-\deltaD relationships between the sub-cloud and cloud layers in StCMBLs with the goal of detecting precipitation in the previous 12-24 hrs. The data show that in most cases, distinguishing precipitation from turbulent mixing between ocean surface evaporation and dry air above the cloud layer requires parsing  $\delta D$ signals of 2-5 permil which is guite small for an aircraft system moving at 130 m/s and measuring at 1 Hz frequency, but is within possibility. There are also several reasons why the isotope measurements are more promising. First, the data show several cases where the data unambiguously follow either a mixing or Rayleigh relationship. Second, for the instances where WISPER sampled StCMBLs transitioning to cumulus-coupled boundary layers,  $\delta D$  variations were greater, at 5-10 permil. Third, we look at a particular case between two days and show that on one day there is evidence of precipitation while in the other there is only mixing and further, the day with precipitation evidence also shows lower aerosol concentration, indicating that we are potentially detecting aerosol scavenging. Ultimately, detailed analyses and integration of isotope data into models with other thermodynamic variables will be required to further constrain moisture and energy budgets in StCMBLs.

#### Development of MIROC5-iso and its comparison with isotopic climate proxies

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Proxy system models (PSMs) are an essential bridge between climate simulations and climate records prior to the period where instrumental observations are available. PSMs help to interpret what proxies show and how they record climate. Although previous studies have evaluated PSMs for individual sites, their systematic evaluation on a global scale has not been conducted. This study evaluated the performance of PSMs for stable water isotopes in ice cores, corals, and tree-ring cellulose for the period 1950–2007. We used a newly developed isotope-enabled atmospheric GCM named MIROC5-iso to provide input data for the PSMs. MIROC5-iso was nudged toward NCEP/NCAR Reanalysis to synchronize the model with the nature. The evaluation result shows that the mean state and the variability were generally well simulated for all proxy types. However, the reproducibility of interannual variability in ice cores was markedly lower. Although the reproducibility was limited by the atmospheric forcing used to drive the model, the results suggest that the PSM may be missing post-depositional processes, such as sublimation for ice cores on the interannual time scale.

In the presentation, our recent progress in developing a new isotope-enabled CGCM named MIROC6-iso will also be introduced.

#### Estimation of monsoon withdrawal date in southern India using the isotopic technique

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Oxygen and hydrogen isotopic ratios in rainfall show strong seasonal variability in the southern parts of India. Such a contrast in isotopic values arises mainly because of the seasonal reversal of the monsoon winds. During the summer monsoon season, the Arabian Sea transports moisture, while during the winter, it is sourced primarily from the Bay of Bengal and the adjoining maritime continents. Atmospheric processes also contribute to these differences. We collected precipitation samples from a southern Indian site (Trivandrum) and two neighboring island sites (Minicoy Island in the Arabian Sea and the Andaman Islands in the Bay of Bengal) to study their seasonal characteristics. The sampling period ranged from 2015 to 2020. We generated a total of eleven oxygen isotopic time series of rainfall approximately from June to December.

Oxygen isotopic values showed a strong association with the Webster-Yang monsoon circulation index. Two distinct clusters were formed when the oxygen isotopes were plotted against the above-mentioned monsoon index. The formation of clusters appears to show the precipitation isotopes' response to moisture dynamics, which significantly changed during the transition phase of the southwest to the northeast monsoon. A strong isotopic seasonality provided us with an opportunity to estimate the summer monsoon withdrawal date in this region. The calculated dates matched well with the estimates based on another method that relied on the thermodynamic characteristics of the atmosphere.

### Examination of the influence of shallow convective mixing on low-level clouds with observations of stable water isotopes

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Low-cloud feedbacks contribute large uncertainties to climate projections and estimated climate sensitivity. A key physical process modulating low-cloud feedbacks is shallow convective mixing between the boundary layer and the free troposphere. However, there are challenges in acquiring observational estimates of shallow convective mixing with global coverage. To this end, we propose a novel approach to constraining convective mixing using stable water vapor isotope profiles from satellite retrievals. We demonstrate that the vertical gradient of water vapor  $\delta D$  between the boundary layer and free troposphere can be used to track shallow convective mixing. Analyzing isotopes in water vapor alongside low-cloud properties from satellite retrievals, we find that low-cloud fraction appears insensitive to convective mixing in shallow cumulus regions. Our results suggest that the relationship between the satellite-derived observations of shallow convective mixing is associated with the moistening of the free troposphere in the tropics. The new estimate of shallow convective mixing with low-cloud properties house potential to validate the simulation of low-cloud feedbacks, refining estimations of climate sensitivity.

### From atmospheric water isotopes measurement to snow core interpretation in Adelie Land: A case study for GCMs with embedded isotopes in Antarctica.

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It is key to estimate the evolution of the atmospheric hydrological cycle in the polar regions, which directly influences the surface mass balance of the Arctic and Antarctic ice caps. Records are available from satellite data for the last 50 years and a few rare weather data since the 50's in Antarctica. One of the best ways to access longer records is to use climate proxies in snow cores. The water isotopic composition in these cores is widely used to reconstruct past temperature variations. However, the link between temperature and isotopic composition is not very well constrained because many other parameters influence the isotopic composition of snow at the time of its formation or after snow deposition on the surface. We need to better understand the atmospheric hydrological cycle and its influence on the isotopic composition of vapour and precipitation in polar regions with the idea of improving the interpretation of snow core records in these regions.

We first present time series of vapor and precipitation isotopic composition measurement at Dumon D'Urville station. Thanks to new technical solution, we were able to measure the vapor isotopic composition all year round in Antarctica. This unique series would make possible to document the isotopic signature of the atmospheric hydrological cycle in Terre Adélie. Then, this data set is used to evaluate GCMs (LMDZ-iso and ECHAM-wiso) in a region where local condition (i.e. strong katabatic wind) directly impacts the isotopic signal. Showing that models with water stable isotopes embedded are likely to reproduce observations, we estimate the signal recorded in Adelie land through a synthetic snow core made from model outputs. Finally, we compare synthetic record to recently drilled cores from the ASUMA program. Preliminary results show that temperature, main post-deposition process (i.e. isotopic diffusion) and precipitation intermittency are not able to fully understand the signal recorded. This new comparison between in-situ measurement and model-based snow core open perspective for the interpretation of isotopic climate proxy in Adelie Land.

High-resolution, near-surface profiles of stable water isotopes over snow-covered tundra and fjord water

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The hydrological cycle is a large source of uncertainty in numerical weather and climate modelling. One cause is that sub-grid scale processes, such as evaporation and precipitation, can lead to unnoticed compensating errors. These processes can be studied with stable water isotopes (SWI), as they are an integrated tracer for the phase changes that atmospheric moisture has undergone. Ny Ålesund is ideally situated for investigations as water vapour observed there can be from local evaporation produced during cold air outbreaks, representing the start of the atmospheric water cycle in the arctic.

The ISLAS2020 measurement campaign during Feb-Mar 2020 in Ny-Ålesund primarily focused on evaporation and vapour deposition processes. During a three week period, under very cold and dry conditions (below -20°C), we obtained multiple near-surface SWI profiles (<5 m). Profiles were made over open water and snow-covered tundra, by way of a SWI analyser in a prototype deployment and profiling system. Installed nearby at both deployment locations were fiber-optic distributed sensing columns, supplying high-resolution temperature profiles (~2 m) above the snow/water. Our tundra site was also chosen to be in the vicinity of a four-level automated weather station, providing valuable wind information to accompany our isotope profiles. The evolution of the underlying surface was monitored by way of sampling the fjord water/snowpack multiple times during profiling. Our near-surface profiles have captured the mixing of two end-members of arctic moisture: Less depleted water vapour originating from the partially ice-covered fjord, and strongly depleted air dried by intense cooling and condensation over the terrestrial snowpack. Their incomplete mixture establishes strong vertical gradients in both the main isotopes, and the deuterium excess.

The stable water isotope observations collected during ISLAS2020 have resulted in a unique dataset of the Arctic water cycle. Observations from the campaign will serve as a basis for ongoing work focusing on the remaining stages of the hydrological cycle. Such work includes isotopic connections on the synoptic scale via Lagrangian transport model (FLEXPART), which can link Ny-Ålesund observations with precipitation sampling at downstream locations, such as Longyearbyen, Tromsø, Andenes, Ålesund, and Bergen.

#### Impact of convective organization on tropospheric humidity and isotopic composition

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Deep convection in the tropics can take the form of small isolated cumulonimbus, or organize into bigger and longer-lived convective systems, such as squall lines or tropical cyclones. Convective aggregation measures the degree to which convection is clustered into a small number of systems. It has already been shown that over the oceans, for a given rain rate in average over some large-scale domain (a few degrees), the troposphere is drier when convection is more aggregated. It has been suggested that the smaller surface of exchanges between clouds and their environment, or the larger fraction of the domain far from clouds, explain the drying. If convective aggregation is effectively responsible for the drying (and not just a consequence of large-scale conditions favoring drying) and if it depends on sea surface temperature, it could be involved in a climate feedback that is not accounted for in global climate models.

In this study, we set two questions : (1) Do aspects of convective organization other than aggregation covary with tropospheric humidity ? (2) What are the mechanisms (convective or large-scale) underlying the organization-humidity relationships ?

(1) Do other aspects of convective organization, such as the life duration of convective systems, their propagation speed or mesoscale dyanmics, also covary with tropospheric humidity ? To address this issue, we co-locate humidity measurements from AIRS with the density and properties of convective systems from the mesoscale convective system tracking algorithm TOOCAN, over tropical oceans during 2012-2016. We find that although convective aggregation is the main factor affecting troposperic humidity, for a given rain rate and density of convective systems, the troposphere is also moister as systems live longer and propagate faster, especially in the upper troposphere. It is also associated with a larger proportion of stratiform rain (observed by TRMM) and a larger ice cloudiness (observed by CALIPSO-Cloudsat).

(2) What mechanisms explain the relationships between troposheric humidity and convective organization ? Large-scale conditions associated with different convective organization states are investigated using ERA5 reanalyses. We find that large-scale vertical and horizontal advections are not major drivers of organization-humidity relationships, except for a significant (but not dominant) effect of top-heavy ascent on the moister troposphere for longer-lived and faster-propagative systems. This suggests that convective processes are responsible for organization-humidity relationships.

The water vapor isotopic composition is used to investigate these processes. The isotopic signature of convective processes in different organized convective systems (squall lines, tropical cyclones) are first investigated in cloud resolving simulations. We find that rain evaporation, especially for stratiform rain, has a strong depleting effect. Coming back to observations, we investigate joint humidity-isotope relationships from AIRS associated with different convective organization states. We find that the moister troposphere in disaggregated states is associated with greater rain evaporation, consistent with the larger surface of exchanges between clouds and their environment. We also find that the moister troposphere around longer-lived convective systems is associated with greater rain evaporation and convective or mesoscale downdrafts, consistent with the greater proportion of stratiform rain, especially for tropical cyclones.

### In-situ vapor isotope measurement in the Arctic seas (Summer 2018): links to moisture origin at synoptic time scales?

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Local evaporation in the Arctic is likely to increase with sea-ice retreat in the context of climate change. In parallel, the transport of moisture from the North Atlantic may also increase, especially in cases of weak polar vortex, associated to blocking over the Norwegian Sea and fast vapor transport into the Arctic. In order to evaluate the contribution of different sources to the moisture budget in the Arctic, a tool is needed to track the transport of vapor in the region.

Here, we combine in-situ measurements of vapor isotope composition to analysis of backtrajectories, to reconstruct the pathway of vapor transport in different synoptic situations during two cruises North of Svalbard in 2018 and 2019 (INTAROS campaigns). We contrast Atlantic (southerly) air masses and Arctic (northerly) air masses, based on the main isotope parameter dD, which quantifies the degree of distillation of air masses after evaporation. An atmospheric river is sampled on the 29th of August 2019, that shows that Atlantic air is characterized by high humidity and high dD values, opposite to Arctic air. In addition, high dD values are observed in air coming from Europe during the very hot summer of 2018. We also measure the secondary parameter dexcess, which varies with evaporation conditions at the source. We find a high d-excess in air from the western arctic, indicative of evaporation at low relative humidity, probably in Cold Air Outbreak situations. Oppositely, we find a relatively low d-excess in air coming from the Barents Sea.

This study highlights the potential of isotopes for identifying moisture sources around the Arctic. However, a full budget for moisture will require simultaneous measurements of vapor around the Arctic, through international collaborations. Moreover, isotope-enabled models, as well as satellite observations of vapor dD values, will also be important to understand the processes causing differences in isotopes, and to provide a statistical overview of the various contributions.

#### Inferring global-scale spatio-temporal δ18OP patterns from local datasets

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Characterising variability in the global water cycle is fundamental to predicting impacts of future climate change. Water isotopes are ideal tracers of spatio-temporal variability within the global water cycle, because they retain information about circulation-dependent processes including moisture source, transport, and delivery.  $\delta$ 180 has been measured in precipitation since the 1950s, and tens of thousands of precipitation  $\delta$ 180 ( $\delta$ 180P) measurements are freely available from the Global Network of Isotopes in Precipitation database (GNIP) and other online repositories (e.g. Bowen et al. 2019; Putman and Bowen 2019). But the spatial coverage of  $\delta$ 180P datasets is patchy, and temporal coverage is irregular and often discontinuous even at individual sites. This has limited characterisation of global-scale spatio-temporal  $\delta$ 180P variability.

Here we collated publicly-available measurements of  $\delta$ 18OP, and employed a novel 'dynamic compositing' technique to synthesise long (34-year), globally-distributed composite records from temporally discontinuous  $\delta$ 18OP measurements. We investigated relationships between global-scale  $\delta$ 18OP variability and various globally-relevant modes of climate variability, including the El Niño Southern Oscillation (ENSO), the Pacific Walker circulation (PWC), and global mean temperature (GMT). We also used isotope-enabled climate model simulations to assess potential biases arising from uneven geographical distribution of the observations or our data processing methodology.

Co-variability underlying the  $\delta$ 18OP composites is more strongly correlated with the PWC (r = 0.74) than any other index of climate variability tested. We propose that the PWC imprint in global  $\delta$ 18OP arises from multiple complementary processes, including PWC-related changes in moisture source and transport length, and a PWC- or ENSO-driven 'amount effect' in tropical regions. The clear PWC imprint in global  $\delta$ 18OP implies a strong PWC influence on the regional expression of global water cycle variability on interannual to decadal timescales.

# Inter-comparison of water isotope-enabled models and reanalysis nudging effects: step forward in SWING project

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The Stable Water Isotope Intercomparison Group (SWING) phase 1 (Werner, 2004) and phase 2 (Risi et al., 2012) were comparison projects across the water isotope-enabled Atmospheric General Circulation Models (AGCMs). The results, openly accessible, have been extensively used by the water isotopes communities. However, the simulations under this framework have been performed with different parameterizations, different forcings, and nudged or not by different reanalysis datasets. Then, a more uniform experimental design is required to interpret rigorously. Therefore, we performed three numerical models NDSL-IsoGSM (Yoshimura et al., 2008) (Chang & Yoshimura, 2015), MIROC5-iso (Okazaki & Yoshimura, 2019), and ECHAM6-wiso (Cauquoin et al., 2019) available in our team in order to make the first home-made intercomparison for water isotope-enabled models.

Our study is divided into two parts: (1) to evaluate the strengths and the weaknesses of these models by reproducing the spatial and temporal variations of observed isotopic signals for the present-day historical period (1979-2020); (2) to evaluate the effects of multiple reanalysis datasets used for nudging on our isotope results. For the first part, the temperature and wind fields of the three AGCMs are nudged to a single dataset, JRA55 (Kobayashi et al., 2015). In addition, the sea surface temperature and the sea ice fields are also provided to the models. For the second part, we performed simulations using different reanalysis datasets JRA55, NCEP-R2 (Kanamitsu et al., 2002), and ERA5 (Hersbach et al., 2020) for a single model, NDSL-IsoGSM. Stable Water Vapor Isotope Database (Wei et al., 2019), Global Network of Isotopes in Precipitation (IAEA/WMO) surface data, and Tropospheric Emission Spectrometer (NASA) satellite vertical data are used to assess the performance of our models, including the fractionation processes of water isotopes.

We obtained diverse results among our simulations, especially inland. The most distinct intermodel spread for  $\delta$ 180 in precipitation appears in Antarctica. Other extreme weather areas, such as Greenland, Andes Mountain, Sahara Desert, and Tibetan Plateau, are also remarkable in different time scales. Furthermore, we will discuss the vertical distribution of water isotopes in the atmosphere regarding similarities and differences among our simulations with seasonal variability.

Like SWING projects, the general purpose of this study is to quantify models' uncertainties and make a modeled isotope dataset publicly available. Thus, it stewards a first step for, we hope, a more comprehensive but intense inter-comparison project, stepping forward in the ensemble of the isotope-enabled models for the climate community.

#### Introduction of the new isotope-enabled global water transport model

#### Naoyuki Kurita, Nagoya University, Japan

Accurate simulation of water cycle is vital to replicating observed water isotopologues from the isotope-enabled models. The recent advances of atmospheric reanalysis enabled us to use high quality atmospheric moisture and precipitation data over space and time. This reminds us that atmospheric water budget approach using reanalysis data would reasonably capture the observed water isotopic data. In this presentation, I will present the performance of this new approach and discuss the usefulness of this model.

The basic concept of the model used in this study is global water transport model coupled with hydrological processes. The following hydrological processes are included in the model: large-scale transport, precipitation and convective transport, vertical diffusion, evaporation from the surface, and the land surface processes (vertical soil moisture transport). The model transports water vapor by using the vertically conservative semi-Lagrangian advection scheme fed by atmospheric winds of reanalysis. Then water vapor exceeding humidity content of reanalysis removes as precipitation. The precipitation process is divided into two categories: large-scale condensation and cumulus convection. The water isotopologues are separately treated in the model and their fractionation processes due to condensation and evaporation are incorporated. In this study, the ERA-Interim reanalysis was used as forcing data. The simulation started in January 1979 and was run until 2018.

The results show reasonable replication of the global precipitation isotope pattern except for some of the dry continental area (e.g., eastern Siberia). The simulated precipitation isotopes over the dry continent are lower than the observed data, although precipitation field is almost identical with observations. In this simulation, the partitioning land surface flux into transpiration and surface evaporation was not considered and the isotopic fractionation during the land surface evaporation was also ignored. Thus, we can speculate that soil evaporation plays an important role for local precipitation. This result not only points out the defects of our model, but also shows the usefulness of this approach to identify a key hydrological process at there. The uniqueness of this approach is that the mismatches between models and observations are mainly attributed by isotope physics. Thus, this approach can be used as a tool for development of our isotope physics scheme.

# Investigation of the preservation of the water isotopic moisture source signal in atmospheric vapour, snowfall and snow pack at Finse, Norway during winter season 2018-2019

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Seasonal snow cover is a crucial resource for hydropower in Norway. Understanding water sources and processes related to inter-annual snow cover variability is therefore of fundamental societal relevance. The stable water isotope composition of precipitation provides a natural, integrated tracer of the condensation history during atmospheric water transport. The main parameters dD and d18O along with the secondary quantity d-excess give information about the origin and transport history of moisture from its source to its sink. When snow falls and deposits on the ground as a sediment, it creates a record in the form of the seasonal snow pack.

Here we utilize data acquired during a field campaign in the winter season of 2018-2019 at the Finse Alpine Research Station Center (1222m, 60.6N, 7.5E) in Norway, in order to investigate the transfer and preservation of the isotopic signal of source and transport conditions from vapour to snowfall, and to the snow pack.

Over a main period of two months, snowfall was sampled daily, while the water vapour was continuously measured from ambient air guided through a heated inlet to a Picarro L2130i infrared spectrometer, with daily calibration runs. During five periods with intense snowfall, we carried out higher frequency sampling down to 15 minute intervals. Covering the entire winter season, five snowpits were sampled for isotopic analysis as well as detailed stratigraphy. In total more than 400 snow samples where taken and analysed for their isotopic composition, accompanied by routine meteorological observations over the winter season at the site. In addition, we compare the variations in the observed isotope signal at Finse with one derived from moisture source analysis using the Lagrangian diagnostic WaterSip, based on the FLEXPART model and ERA Interim reanalysis data.

To investigate to what degree moisture source information is archived in the snow pack, and how it evolves during the season, we compare snow observations at different time resolution (daily and high frequency snowfall samples) with the record of the snow pack, aided by the snow model CROCUS. The meteorological observations supply context for understanding the snow formation conditions. In particular, deviations from isotopic equilibrium between vapour and precipitation at ambient temperature conditions provide insight into the dominant condensation regime during different intense observation periods.

#### Isotope Signal Formation in Snow - Insights from the Greenland Ice Sheet

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Two of the main application areas of stable water isotope research are model tracer diagnostics and paleoclimate ice core proxy interpretation. In both fields, snow-atmosphere exchange processes are a part of the system, yet they are being neglected as influential processes in both applications due to comparably small mass transport and the assumption of absence of isotopic fractionation during sublimation and therefore a recycling type of exchange.

Here we show the inaccuracy of the latter assumption by providing evidence of fractionation induced sublimation through a combination of laboratory and field experiments as well as snow surface modeling. We show substantial surface enrichment through sublimation and find that the summer season temporal evolution of the snow surface isotopic composition in between precipitation events can be attributed to surface humidity fluxes. We discuss the nature and underlying physical process of fractionation during sublimation based on observed isotopic composition of snow and vapor samples from the Greenland Ice Sheet and laboratory experiments.

Our results lead to an improved process understanding and ask for the implementation of fractionation during the sublimation process in isotope enabled climate models. This will pave the way for the integration of ice core water isotope records in paleo model validation without the need for paleothermometer calibration functions.

#### Isotopic signals in marine atmospheric cold pools

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Understanding the relationship between trade cumulus clouds and boundary layer humidity is challenging due to the spatial and temporal scales involved in the interactions, and the historical limits in modeling and observations of the contributing phenomena. Here we examine the properties of trade wind boundary layers associated with cold pools. In situ time series measurements of stable water isotopes (HDO and H218O) in the subcloud boundary layer (SBL) were collected aboard a ship during the Atlantic Tradewind Ocean-Atmosphere Mesoscale Interaction Campaign (ATOMIC) in January-February 2020. During this isotope time series, 22 cold pools were identified from the air temperature. In 59% of the cold pools, deuterium (D) concentration increased as the temperature dropped, with stronger spikes in  $\delta D$  corresponding to larger decreases in temperature, especially when precipitation is observed at the ship. A hypothesis for this distinct isotopic signal is that hydrometeors, enriched in D by cloud condensation distillation, mostly evaporate to enrich water vapor in downdrafts, which provides the positive anomaly at ground level detected at the downdraft front. Systematic enrichment of O18 is not observed during cold pools. Consequently, deuterium excess (DXS =  $\delta D - 8\delta O18$ ) is moderate for cold pools (9-11 permil), and is correlated to humidity rather than to temperature. DXS in the SBL is low (6-8 permil) when specific humidity is high (~16 g/kg), associated with surface evaporation at relative humidity (RH) near 80%. Higher DXS (~13 permil) at lower specific humidity (~12 g/kg) suggests the water vapor evaporated at much lower RH from hydrometeors in the cloud layer aloft. In combination with conserved meteorological variables (potential temperature and specific humidity), isotope concentrations suggest which types of evaporation processes affect cold pools and the SBL air.

#### Isotopic signals in precipitation and water vapor during the Hurricanes Irma & Maria

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Stable water isotopes (H216O, HD16O and H218O, expressed hereafter in the usual δ notation) are widely used in meteorological and hydrological studies for their sensitivity to climate parameters like temperature and precipitation amount. They are also used to better understand the mechanisms that control the transport of water vapor caused by different weather patterns, including extreme events such as tropical cyclones (hurricanes/typhoons). It has been shown that global distribution of tropical cyclones has changed in recent years and may in part be attributable to the increase in greenhouse gas emissions. Especially, a substantial increase of the trend in tropical cyclone frequency of occurrence in North Atlantic Ocean has been shown. Therefore, it is of great significance to study on the formation, movement and water origin of the hurricanes in the Atlantic Ocean. In this work, we present isotope-enabled simulations of two recent super-hurricanes formed in open Atlantic Ocean in September 2017, Irma and Maria. We used in-situ observations and two isotope-enabled Atmosphere General Circulation Models (AGCM) nudged to ERA5 reanalyses: high resolution ECHAM6-wiso (approx. 0.9°x0.9° horizontal resolution and 95 vertical atmosphere layers) and lower resolution IsoGSM (approx. 1.9°x1.9° horizontal resolution and 17 vertical atmosphere layers) models.

The comparison between observations and models results indicates that ECHAM6-wiso is able to simulate isotopic ratio in precipitation, but may underestimate the precipitation amount during the passage of the hurricane. The surface vapor  $\delta 2H$  decreased inward toward the center of the hurricane, while the d-excess (d-excess =  $\delta 2H-8 \times \delta 18O$ ) was higher in the center. This phenomenon is consistent with the moisture cycling process in hurricane, where the high condensation efficiency of rainstorms and recycling of isotopically depleted vapor could lead to extremely negative  $\delta$ 2H and a high d-excess in vapor and precipitation. The simulated d-excess in surface water vapor in the hurricanes is higher in ECHAM6-wiso than in IsoGSM, partly due to the difference in modeled specific humidity and latent heat flux values between the two simulations. The spatial resolution is an important factor because it influences the vertical structure of modeled  $\delta 2H$  and d-excess in water vapor and the representation of latent heat flux. Finally, the  $\delta 2H$  in surface water vapor near the Irma hurricane center decreased linearly during the hurricane lifetime. On the other hand, the δ2H signal increased in the last half period of Maria hurricane. According to the modeled moisture flux from ECHAM6-wiso, after moving westward, Irma made a landfall in the US and dissipated quickly. On the other hand, Maria turned toward North and reached the ~40°N latitude. In this case, moisture from low-latitude ocean surface was still transported to the hurricane, which caused this increase of isotopic ratio of surface water vapor in the last half period.

#### Isotopic traits of the Arctic water cycle

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The Arctic hydrological cycle undergoes rapid and pronounced changes, including marine and terrestrial ice loss, increased atmospheric humidity, shifting ocean circulation regimes, and changes in the magnitude and frequency of extreme weather events. Due to the recent reduced sea ice coverage, Arctic-derived moisture serves as a new, increasingly important northern hemispheric water source. Stable water isotopes ( $\delta$ 180,  $\delta$ 2H) and the secondary parameter d-excess can be used to trace the processes within this new evaporative system including the potential feedback of them into the global climate system. However, characteristics of  $\delta$ 180,  $\delta$ 2H and d-excess and the processes governing them are yet to be quantified across the Arctic due to a lack of long-term empirical data. The Multidisciplinary drifting Observatory for the Study of Arctic Climate (MOSAiC) expedition provided a unique opportunity to collect, analyze, and synthesize discrete samples of the different hydrological compartments in the central Arctic, covering a complete seasonal cycle over the course one year. These observations can lead to a new insight into coupled climate processes operating in the Arctic.

Here, we present the isotopic traits of more than 1,900 discrete samples (i.e., seawater, sea ice, snow, brine, frost flower, lead ice, ridge ice). We found that: (i) average seawater  $\delta 180$  of -1.7‰ conforms to observed and modelled isotopic traits of the Arctic Ocean with more depleted seawater closer to the north pole in winter and relatively enriched seawater in lower latitudes in spring; (ii) second year ice is relatively depleted compared to first year ice with average  $\delta 180$  values of -3.1‰ and -0.7‰, respectively. This might be due to post-depositional exchange processes with snow; (iii) snow has the most depleted isotopic signature among all compartments (mean  $\delta 180$ =-15.1‰) and a gradual enrichment trend in snow profiles from top to bottom might be partially due to sublimation of deposited snow.

Our dataset provides an unprecedented description of the present-day isotopic composition of the Arctic water covering a complete seasonal cycle. We try to assess the relative contribution of snow, sea ice, leads, and melt ponds spatially and temporally on regional and local moisture in the Arctic. This will ultimately contribute to resolve the linkages between sea ice, ocean, and atmosphere during critical transitions from frozen ocean to open water conditions.

#### Kinetic fractionation factors for ocean evaporation: limited impact of wind speed observed

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Isotope non-equilibrium fractionation effects are important during ocean evaporation and sensitive to environmental conditions such as temperature and relative humidity in the lower troposphere. Isotopic evaporation models, such as the Craig-Gordon model, rely on the description of nonequilibrium fractionation factors that are, in general, poorly constrained. To date, only a few gradient-diffusion type measurements have been performed in ocean settings to test the validity of the commonly used kinetic fractionation factor parametrizations for ocean evaporation. In this work we present six months of water vapor isotopic observations collected from a meteorological tower located in the northwest Atlantic (Bermuda) with the objective of estimating the best kinetic fractionation factors (k, ‰) for ocean evaporation and their dependency on wind speed. Gradientdiffusion measurements are sensitive enough to resolve kinetic fractionation factors during evaporation and provide mean values of  $k_{18} = 5.2 \pm 0.6$  ‰ and  $k_{2} = 4.3 \pm 3.4$  ‰. In this study, a relationship between k and 10m-wind speed has been observed directly over the ocean. This relationship is expected from current evaporation theory and from laboratory tests made in the 1970s. However, we show that (i) sensitivity of k to wind speed is small, in the order of -0.19 s m-1 for k18, and (ii) there is no experimental evidence for the presence of a discontinuity between smooth and rough wind speed regime during isotopic fractionation. In general, k18 monotonically decreases until wind speed is ~9-10 m s-1.

### Long-term mountain precipitation and stream water isotopes from New Hampshire wilderness; initial results

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The Appalachian Mountain Club (AMC) has been collecting cloud, rain, and stream samples in the White Mountain National Forest (WMNF) in New Hampshire USA at mountain sites for decades and has a sample archive that stretches back to 1995. Samples are collected during the growing season for tracking air pollution in collaboration with the WMNF Clean Air Act monitoring of wilderness air quality related values. Storage of samples is in the original HDPE collection bottles and kept in cool storage at approximately 13-18 degrees C. In recognition of the potential added insights into water and pollution cycles from rain and cloud inputs to stream water, the water isotopic composition of the AMC samples was recently analyzed. Here, we report preliminary results from this exploratory analysis. Water isotopic analysis was conducted on growing season precipitation samples (1996-2016) and the stream and lake water sample archive (1995-1997;2001-2019). No sample evaporation signal was apparent when examining  $\delta$ 180 over time in either precipitation or stream samples. Stream sample sites include a climatic gradient from mid-elevation mix deciduous forest sites to those at treeline and alpine ponds. Using the high elevation (1539 m) rain water a meteoric water line was established ( $\delta D$ = 16.29 + 8.16  $\delta$ 18O). This LMWL was similar to that reported at nearby USFS Hubbard Brook Experimental Forest. Thornton, NH for the 2006-2010 growing season but with a slightly steeper slope; Hubbard Brook LMWL slope: 7.56 (Green et al 2015). d-excess was also calculated as defined by Dansgaard (1964). Results for cloud and rainwater are distinctly different between the AMC's high elevation site and Hubbard Brook rain water, with the former much more depleted than the latter during the growing season, possibly highlighting the role of transpiration in influencing near-surface humidity and precipitation patterns. Air mass mean temperature explains more than a third of the rain and cloud  $\delta$ 180 variability and the relationship improves with partition by westerly wind direction. No relationship of air temperature with d-excess was found. Results for AMC's surface water samples to date had a d-excess inter-quartile range from 11.00-17.25 (values more variable than, but comparable to, stream samples from Hubbard Brook 12.57-16.56) with overall isotopic signatures indicate more of an upper elevation precipitation input signal. Data also suggest depletion in  $\delta$ 180 in surface waters along an elevational gradients with the exception of the highest altitude sites which showed greater variability, including some of the most enriched values. This enriched surface water includes both alpine ponds and headwater streams with the former potentially explained by evaporation. Enrichment in headwater streams may indicate that fresh contributions of precipitation are being measured which is plausible considering lack of tree cover and the steep terrain accommodating expedited runoff.

#### Measuring cloud isotope ratios behind a Counterflow Virtual Impactor

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Fast (> 1Hz) water vapor isotopic analyzers have made it possible to resolve important spatial variability while measuring isotope ratios in water vapor from aircraft moving at speeds exceeding 100m/s. The emergent result is an improved picture of key environmental features, like the atmospheric isotopic vertical profile, which critically informs evaluations of isotopically enabled numerical simulations and HDO satellite retrievals. Fast isotopic analyzers are now being paired with aerial Counterflow Virtual Impactors, or CVIs, that separate cloud droplets and ice from the background water vapor. This combined measurement approach creates exciting new possibilities for evaluating water budgets in the atmosphere and investigating cloud microphysical processes.

Here, we report first measurements from a fast water vapor isotopic analyzer paired with a CVI newly developed for the NCAR/NSF research aircraft. The combined system flew more than 50 research hours during the recent NSF-funded SPICULE mission, whose aim was to study secondary ice formation in cumulus clouds. The flights took place during May and June 2021 and covered the central-southern United States. In addition to showcasing the isotopic data collected in cloud and in background vapor, we also present examples of inlet saturation and sample evaporation during flight in order to highlight the challenge of measuring liquid isotope ratios from aircraft. Such signals also demonstrate the value of using isotopic measurements to improve inlet design and airborne sampling strategies for other cabin-based measurements.

#### MJO/BSISO and Stable isotope variation of precipitation in southern Asia

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MJO and BSISO can significantly affect the intra-seasonal fluctuations of stable isotopes in precipitation in Asian equatorial region and Asian monsoon region during boreal winter and boreal summer respectively. The amplitude of intra-seasonal fluctuations of stable isotopes in precipitation cover those regions are about 10 per mil, and the variation of amplitude is associated with the strength of convection propagating to the region and the elevation of the region.

# Observations and Simulations of the Stable Water Isotope Signature of Convective Updrafts and Downdrafts Associated with Different Mesoscale Organization Patterns of Shallow Trade Wind Clouds

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Each process controlling the water vapor budget of shallow cumulus clouds in the trade wind region such as ocean evaporation, convective and turbulent mixing, condensation and evaporation of hydrometeors is associated with a characteristic isotopic fingerprint. In a recent study, different transport regimes in the trades have been shown to be associated with distinct mesoscale organization patterns and water vapor isotope signals in the sub-cloud layer. The reported isotopic differentiation between various mesoscale organisation patterns is most likely due to variations in the relative contribution of the processes mentioned above to the water vapor budget along the flow. To test this hypothesis and assess the timescales over which the patternspecific anomalies in water vapor isotopes emerge, we use a combination of airborne measurements of stable water vapor isotopes and high-resolution simulations with the isotopeenabled numerical model COSMOiso. The evolution of the stable isotope signature along the trade wind flow is assessed using three-dimensional back-trajectories calculated based on COSMOiso wind fields. The isotope measurements in water vapor were performed on the French aircraft ATR-42 during 18 flights from 25 January to 13 February 2020 as a part of the international EUREC4A field campaign. The flights were conducted over the tropical ocean near Barbados with the aircraft staying predominantly at the height of cloud base. Our isotope measurements reveal substantial differences between flights, which are related to contrasting large-scale flow situations and mesoscale cloud organizations. This study provides promising process-based insights into the cloud-circulation coupling conundrum and demonstrates the potential of water isotopes to identify relevant processes.

#### Preliminary results of an isotope-enabled earth system model AWIESM-wiso

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We show here the first results of two equilibrium simulations under pre-industrial (PI) and Last Glacial Maximum (LGM) boundary conditions, using a state-of-the-art earth system model (AWIESM-wiso) equipped with water stable isotopes. The model applies a full free surface formulation which enables a more realistic handling of freshwater fluxes, sea level and ocean volume changes. Variable resolution up to 12 km is implemented in the ocean module. Our model shows a good match between the simulated and observed delta180 in precipitation in the PI. The modeled heavy isotope ratios in both surface sea water and interior ocean, are in good agreement with foraminifera-based records. Colder and dryer climate is represented in the LGM as compared to PI, consistent with various archives and PMIP-model ensemble patterns. We find a high correlation between the simulated and reconstructed anomalous delta180 in precipitation (LGM-PI) at sites of Antarctic ice cores and sub-tropical speleothems. The positive anomalies in delta180 in sea water, with the magnitudes being 1.5-2 permil for Atlantic section and 1-1.6 permil for Pacific section as evidenced in benthic foraminifera data, are well captured by our model.

#### Probing the Trade-Regime Water Cycle: Comparing Isotopes, Soundings, and Surface-Based Remote Sensing Aboard the RV Meteor during EUREC4A

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The EUREC4A field campaign during early 2020 gathered comprehensive measurements of the exemplar trade-wind region east of Barbados to better understand the coupled relationships between moisture, circulation, and low clouds in the tropical marine atmospheric boundary layer. This included the EUREC4A-iso effort with extensive measurements of vapor, rain, and seawater isotopic composition from land, sea, and airborne platforms. A critical question is what balance of processes controls the moisture budget, particularly of the subcloud layer. Changes in the oceanic moisture flux can be difficult to disentangle from convective mixing, and exchanges with the free troposphere. Cold-pools have also been found as a dominant driver of both moisture variability and low-cloud behavior. Since the trade-cumulus regime boundary layer is often decoupled, the negative buoyancy required for downdrafts is primarily achieved through precipitation evaporation, further modifying near-surface humidity. Being sensitive to phase change and mixing, isotopic measurement represent a potential way to constrain these processes.

Here we present the isotopic datasets collected aboard the RV Meteor during EUREC4A, as well as two avenues of analysis. The isotopic measurements include 43 days of continuous vapor measurements, rain samples from 15 rain events, and near-daily surface seawater samples. A first analysis approach uses a set of simple model calculations, constrained by sea-surface and sounding measurements, to estimate plausible sources of near-surface moisture. Here the mixing framework proposed by Benetti, et al. (2015, 2018) is used to show that a closure assumption oceanic flux subjected to a small amount of Rayleigh-like condensation in the local cloud layer is sufficient to explain the distribution of data. A second approach leverages the vertical cloud Doppler radar and microwave radiometer humidity profiles to observe cloud extent and estimate precipitation evaporation between the cloud-base and surface. Variations in vertical and horizontal cloud extent are found to correlate with distinct patterns in near-surface water vapor  $\delta 180$ ,  $\delta D$ , and Deuterium-excess. The isotopic response and surface meteorology before, at onset, and during precipitation events is cataloged revealing differing temporal patterns for highly evaporative virga versus surface-reaching precipitation.

# Quantifying ET Over the Congo Basin Using a Combination of Remotely-sensed and Surface Measurements

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The Congo Basin hosts the driest rainforest in the world, with large uncertainties in rainfall. Determining the contributions of free-tropospheric moisture is therefore key for developing a better understanding of the relative influences on precipitation from external SSTA, internal land vegetation, and land-use changes. Bailey et al., (2017) found a linear relationship between net of evapotranspiration minus precipitation (ET-P) and the deuterium content of water at a specific humidity of 4 mmol/mol (dd04), on a tropical scale. Based on their finding, we apply a terrestrial water balance approach to derive ET over the Congo Basin between 2005-2016 using a suite of independent observations, i.e., AIRS deuterium measurements, the Tropical Rainfall Measurement Mission (TRMM) precipitation data, SO-HYBAM river discharge and changes in terrestrial water storage derived by the Gravity Recovery and Climate Experiment (GRACE). We show that ET derived from this approach is greater than atmospheric moisture convergence in all seasons and highest in the rainy seasons. Furthermore, the interannual variation of ET is relatively decoupled with that of rainfall. This result implies a potential resilience of ET, presumably rainforests, to interannual rainfall anomalies.

# Retrieving H2O/HDO columns over cloudy and clear-sky scenes from the Tropospheric Monitoring Instrument (TROPOMI)

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This contribution presents an extended scientific HDO/H2O column data product retrieved from short-wave infrared (SWIR) measurements by the Tropospheric Monitoring Instrument (TROPOMI) including clear-sky and cloudy scenes. The retrieval employs a forward model which accounts for scattering, and the algorithm infers the trace gas column information, surface properties and effective cloud parameters from the observations. The extension to cloudy scenes greatly enhances coverage, particularly enabling data over oceans as the albedo of water in the SWIR spectral range is too low to retrieve under cloud-free conditions. The new data set is validated against co-located ground-based Fourier transform infrared (FTIR) observations by the Total Carbon Column Observing Network (TCCON). The median bias for clear-sky scenes is 1.4 × 10<sup>21</sup> molec/cm<sup>2</sup> (2.9 %) in H<sub>2</sub>O columns and  $1.1 \times 10^{17}$  molec/cm<sup>2</sup> (-0.3 %) in HDO columns, which corresponds to -17 % (9.9 %) in a posteriori  $\delta D$ . The bias for cloudy scenes is  $4.9 \times 10^{21}$  molec/ cm<sup>2</sup> (11 %) in H<sub>2</sub>O,  $1.1 \times 10^{17}$  molec/cm<sup>2</sup> (7.9 %) in HDO, and -20 ‰ (9.7 %) in a posteriori  $\delta$ D. At low-altitude stations in low and middle latitudes the bias is small, and has a larger value at high latitude stations. At high altitude stations, an altitude correction is required to compensate for different partial columns seen by the station and the satellite. The bias in a posteriori  $\delta D$  after altitude correction depends on sensitivity due to shielding by clouds, and on realistic prior profile shapes for both isotopologues. Cloudy scenes generally involve low sensitivity below the clouds, and since the information is filled up by the prior, it plays an important role in these cases. Over oceans, aircraft measurements with the Water Isotope System for Precipitation and Entrainment Research (WISPER) instrument from a field campaign in 2018 are used for validation, yielding a bias of -3.9 % in H<sub>2</sub>O and -3 ‰ in  $\delta$ D over clouds. To demonstrate the added value of the new data set, a short case study of a cold air outbreak over the Atlantic Ocean in January 2020 is presented, showing the daily evolution of the event with single overpass results.

# Stable Water Isotope Incorporation in the Joint UK Land Environment Simulator (JULES) Model

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In our ongoing recent study, we aim to incorporate stable water isotopes into the Joint UK Land Environment Simulator (JULES) model in order to investigate abrupt climate shifts that occurred in the Earth's past climate system. The JULES model is a community land surface model that represents terrestrial processes including surface energy balance, hydrological cycle, carbon cycle, and dynamic vegetation.

We intend to employ stable isotopes of water (HDO and H218O) in the model because they provide insight into the links between various pathways of the global hydrological cycle and climate system processes. As they are powerful tracers of water sources, their ratios and variations can be used to: i) diagnose the implications or causes of changes in hydrological processes, ii) infer information about the history of water while it passes through the hydrological cycle, and iii) interpret paleoisotope records. Due to having slightly different physicochemical properties and different latent heat requirements for phase changes, stable water isotopes vary in their relative abundances among hydrological pools.

In the first stage of our model code development, we will add non-isotopic water tracers to the model, which track prognostic water variables through the hydrological cycle. In the following stage, we will implement in the model code the isotopic fractionation processes that occur during soil and water evaporation, condensation, snow sublimation, and evapotranspiration to convert non-isotopic water variables into stable water isotopes. This implementation will be made and tested in both the standalone and the coupled configurations of the JULES model. The coupled configuration is the land surface component of the isotope-enabled version of the UK Earth System Model (UKESM2), which also consists of an atmosphere model (UM), an ocean model (NEMO), and a sea ice model (SI3). Details of the ongoing developments on the UM model code can be found in a companion poster by McLaren et al.

Our work falls under the large multi-institutional EU Tipping Points in the Earth System (TiPES) project and is expected to be completed by the end of 2022.

# Stable water isotope signals in tropical ice clouds in the West African monsoon simulated with a regional convection-permitting model

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Tropical ice clouds have an important influence on the Earth's radiative balance. They often form as a result of deep convection, which strongly affects the water budget of the tropical tropopause layer. Ice cloud formation involves complex interactions on various scales, which are not fully understood yet and lead to large uncertainties in climate predictions. In this study, we investigate the processes related to ice clouds in the West African monsoon using stable water isotopes as tracers of moist atmospheric processes. We performed simulations using the regional isotopeenabled model COSMOiso with different resolutions and treatments of convection for the period of June-July 2016. First, we evaluate the credibility of our simulations by comparing the isotopic composition of monthly precipitation to GNIP observations, and the temporal evolution of monsoon precipitation to insights from the DACCIWA field campaign in 2016. Next, a case study of a mesoscale convective system (MCS) explores the isotope signatures of tropical deep convection on atmospheric water. Convective updrafts within the MCS inject enriched ice into the upper troposphere at the expense of vapour that is isotopically depleted within these updrafts due to the preferential condensation and deposition of heavy isotopes. Water vapour in downdrafts within the same MCS are enriched by non-fractionating sublimation of ice. In contrast to ice within MCS core regions, ice in widespread cirrus cloud shields is isotopically in approximate equilibrium with the ambient vapour, which is consistent with in situ formation of ice under equilibrium fractionation. These findings from the case study are supported by a statistical evaluation of isotope signals in ice clouds in the African monsoon. The following five key processes related to tropical ice clouds can be distinguished based on their characteristic isotope signatures: (1) convective lofting of enriched ice into the upper troposphere, (2) cirrus clouds that form in situ from ambient vapour under equilibrium fractionation, (3) sedimentation and sublimation of ice in the mixed-phase cloud layer of convective systems and underneath cirrus shields, (4) downward transport of ice in convective downdrafts that sublimates and enriches the environmental vapour, and (5) the freezing of liquid water in the mixed-phase cloud layer at the base of convective updrafts. Importantly, the results show that convective systems strongly modulate the humidity budget and the isotopic composition of the lower tropical tropopause layer. They contribute to about 40% of the total water and 60% of HDO in this region according to estimates based on our model simulations. Overall, this study demonstrates that isotopes can serve as useful tracers to disentangle the role of different processes in the Earth's water cycle, including convective transport, ice cloud formation, and their impact on the tropical tropopause layer.

# Sublimation origin of negative deuterium excess observed in snow and ice samples from McMurdo Dry Valleys and Allan Hills Blue Ice Areas, East Antarctica

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The oxygen and hydrogen isotopic composition ( $\delta$ 180 and  $\delta$ D values) in snow and ice have long been utilized to reconstruct past temperatures of polar regions. Embedded in this approach is an assumption that post-depositional processes such as sublimation do not impact the isotopic composition of snow—an assumption that has been recently questioned. In areas near the McMurdo Dry Valleys in Antarctica, for example, where the accumulation rate is smaller than 0.01 m yr-1, surface snow and ice samples are characterized by a negative deuterium excess ( $\delta D$  - $8^{*}\delta$ 180). This unique phenomenon, only observed near the Dry Valleys, raises the possibility that sublimation may be capable of altering the isotopic composition of the surface snow. Here we use both an isotope-enabled general circulation model and an ice physics model to investigate the origin of these negative deuterium excess values. Our results suggest that negative deuterium excess values can only arise from precipitation if all the moisture is sourced from the Southern Ocean. However, the model results show that moisture sourced from oceans north of 55° S contributes significantly (>50%) to precipitation in Antarctica in the present day. While this contribution likely changes in different climates, it is likely a persistent feature of Antarctic precipitation. We thus propose that sublimation must have occurred to yield the negative deuterium excess values in snow observed in and near the Dry Valleys and that self-diffusion in ice grains is sufficiently fast to allow Rayleigh-like isotopic fractionation in similar environments. We calculate that under present-day conditions at the Allan Hills outside the Dry Valleys, 3 to 24% of the surface snow is lost due to sublimation. Because a higher fraction of snow is expected to be sublimed when accumulation rates are lower, the magnitude of  $\delta 180$  and  $\delta D$  enrichment due to sublimation will be higher during past cold periods than at present. This sensitivity of the snow isotopic composition to accumulation rates and sublimation implies that the cooling in glacial periods could be underestimated if the modern spatial relationship between temperature and precipitation  $\delta D$  and  $\delta 180$  values is applied in cases where no independent temperature calibration is available.

# Synoptic variability of specific humidity and isotope composition over the subtropical North Atlantic: a numerical modelling study

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Due to its dryness, the subtropical free troposphere plays a critical role in the radiative balance of the Earth's climate system. The complex interactions of the dynamical and physical processes controlling the variability in the moisture budget of this sensitive region of the atmosphere, however, are still not fully understood. In this study, we investigate the fundamental characteristics of the subtropical water cycle over the eastern North Atlantic during the West African monsoon season with the aid of the regional weather prediction model COSMO that has been equipped with stable water isotopes and passive water vapour tracers. The water budget for the subtropical mid troposphere is decomposed based on tagged water tracers that represent moisture originating from specified source regions. The analysis reveals two contrasting moisture circulation regimes, resulting from an alternation of dry, isotopically depleted air from the upperlevel extratropical North Atlantic and humid, enriched air from North Africa. This African air is always composed of moisture from mixed sources, which has been advected at low levels into the Saharan heat low (SHL), dry convectively lifted to higher altitudes and eventually transported within the Saharan air layer over the North Atlantic. The employed water vapour tagging approach gives insights into mixing processes along the large-scale transport pathway of atmospheric moisture and notably into the key role of the SHL for understanding the moisture budget in this region during the monsoon season. Considering the entire model domain, the combination of passive water vapour tracers and stable water isotopes can provide a direct link between the evaporative origin of moisture and its isotope signature. We find high correlations of isotope signals with certain passive tracers in the middle troposphere over the eastern subtropical North Atlantic and the western Sahel. However, over the extratropical North Atlantic and the Sahara these correlations are weaker implying that the isotope signals in these regions cannot indicate on the moisture origin.

# The global multi-anual MUSICA IASI {H2O,deID} data product and satellite data perspectives in Europe

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We present the recently published MUSICA IASI {H2O, $\delta$ D}-pair data set consisting of almost 1.5 billion individual data points and offering twice daily global coverage for the October 2014 to December 2020 period. We document the uniqueness of these product with regard to horizontal and global coverage and discuss their application in the field of weather and climate research.

In addition we briefly discuss upcoming possibilities: (1) A MUSICA reprocessing of IASI data a global daily water vapour isotopologue data set covering almost 15 years (2007-present) could be generated. (2) The synergetic combination of the MUSICA IASI and the TROPOMI water vapour isotopologue data would offer perspectives for a global and daily remote sensing of tropospheric water vapour isotopologue profiles (in the near future IASI and TROPOMI successor instruments will by on the same satellites).

#### The Introduction of Stable Water Isotopes to the UK Earth System Model (UKESM2)

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Work has recently started to introduce stable water isotopes to the UK Earth System Model (UKESM2) as part of the EU Tipping Points in the Earth System (TiPES) project. Stable water isotopes are a valuable diagnostic tool in a coupled climate model and there are several potential uses of this development. These include the ability to evaluate past climate model simulations with isotopic measurements from ice cores and to investigate the hydrological cycle of the model.

The physical component of UKESM2 comprises an atmosphere model (UM), an ocean model (NEMO), a sea ice model (SI3) and a land surface model (JULES). This poster describes the general project with a focus on the atmospheric work. A companion poster by Gorguner et al. describes the work being done on the land surface model.

Water isotopes are affected by the same dynamical, physical and biological processes that act on all water species. Therefore, the first stage of this development is to add an array of non-isotopic water tracers to the coupled model, which undergoes the exact same processes as water. In the atmosphere model, the water tracers are affected by the following processes: surface exchange; boundary layer mixing; convection; advection by the large-scale circulation; and microphysical processes in the clouds. The next model development stage is to convert the non-isotopic water tracers to water isotopes by modelling fractionation processes during certain phase changes. In the case of the atmosphere model, fractionation will occur during condensation of water vapour to liquid or ice condensate, in evaporation of liquid condensate and during surface evaporation. Finally, the isotopic fractionation that occurs between rain droplets and water vapour during rainfall (due to evaporation and exchange) will also be included. A development plan for this work will be presented, with anticipated timescales for each step. The aim is to complete the development by the end of 2022.

#### The isotopic composition of rainfall on a subtropical mountainous island

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Tropical islands are some of the most biodiverse and, at the same time, vulnerable places on the planet. Water resources are one of the key players in the equilibrium on which the ecosystems and the population of tropical islands rely. Stable water isotopes have proved to be powerful tools in the study of the hydrometeorology of tropical islands, although the scarcity of long-term and high-frequency data often complicates data interpretation. Here, we present a new dataset consisting of weekly rainfall data collected over a two-year period starting in July 2019 in five different locations across the island of O'ahu. By analyzing the weather conditions during the collection period, we determine the isotopic composition associated with different synoptic systems, like cold fronts and Kona lows, that affect the Hawaiian Islands. The data also shows significant differences between the rainfall isotopic composition on the windward and on the leeward side of the island due to differences in rain evaporation rates. Using trajectory analysis, we also determine the different origins of air masses throughout the year and use this to explain differences in deuterium excess observed in rainfall. Finally, the interannual variability of rainfall isotopes and its large-scale drivers are discussed.

# The role of dew and radiation fog inputs in the local water cycling of a temperate grassland during dry spells in central Europe

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During dry spells, non-rainfall water (hereafter NRW) mostly formed from dew and fog potentially plays an increasingly important role in temperate grassland ecosystems with ongoing global warming. Dew and radiation fog occur in combination during clear and calm nights, and both use ambient water vapor as a source. Research on the combined mechanisms involved in NRW inputs to ecosystems is rare, and distillation of water vapor from the soil as a NRW input pathway for dew formation has hardly been studied. Furthermore, eddy covariance (EC) measurements are associated with large uncertainties on clear, calm nights when dew and radiation fog occur. The aim of this paper is thus to use stable isotopes as tracers to investigate the different NRW input pathways into a temperate Swiss grassland at Chamau during dry spells in summer 2018. Stable isotopes provide additional information on the pathways from water vapor to liquid water (dew and fog) that cannot be measured otherwise. We measured the isotopic composition ( $\delta$ 180,  $\delta$ 2H, and d =  $\delta 2H - 8 \cdot \delta 18O$  of ambient water vapor, NRW droplets on leaf surfaces, and soil moisture and combined them with EC and meteorological observations during one dew-only and two combined dew and radiation fog events. The ambient water vapor d was found to be strongly linked with local surface relative humidity (r = -0.94), highlighting the dominant role of local moisture as a source for ambient water vapor in the synoptic context of the studied dry spells. Detailed observations of the temporal evolution of the ambient water vapor and foliage NRW isotopic signals suggest two different NRW input pathways: (1) the downward pathway through the condensation of ambient water vapor and (2) the upward pathway through the distillation of water vapor from soil onto foliage. We employed a simple two-end-member mixing model using  $\delta$ 18O and  $\delta$ 2H to quantify the NRW inputs from these two different sources. With this approach, we found that distillation contributed 9-42% to the total foliage NRW, which compares well with estimates derived from a near-surface vertical temperature gradient method proposed by Monteith in 1957. The dew and radiation fog potentially produced 0.17–0.54mmd-1 NRW gain on foliage, thereby constituting a non-negligible water flux to the canopy, as compared to the evapotranspiration of 2.7mmd-1. Our results thus underline the importance of NRW inputs to temperate grasslands during dry spells and reveal the complexity of the local water cycle in such conditions, including different pathways of dew and radiation fog water inputs.

# The stable isotopic complexity of thunderstorm precipitation – First results of the IAEA HiRise21 experiment

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Stable hydrogen (2H) and oxygen (18O, recently also 17O) isotopes of precipitation at any given site construe an indispensable input function for hydrological and climatological studies. Traditionally, their interpretation has relied on the explanatory power of air temperature or precipitation amount based on analyses of monthly integrated composite samples. More recent approaches attempted to categorize the stable isotopic composition (including 17O) based on the integration of individual precipitation or storm events and the origin of the air masses where it is distinguishable using the deuterium excess values ( $d=\delta 2H-8^*\delta 18O$ ). However, the microphysical cloud processes generating precipitation are now recognized to be important, as well as partitioning rain events into a dual schema of convective and cyclonic precipitation. Another complication for the interpretation of d-excess, is the extent of sub-cloud evaporation, especially of small raindrops on their downward travel. However, any attempt to disentangle these factors mandates a high temporal resolution of the isotopic and related information.

The IAEA HiRise21 (High-Resolution Isotope Sampling Experiment 2021) was designed to apportion the influences of vapour source region on the precipitation process as well as subcloud evaporation over the May-October 2021 summer/fall period. At the study site in Vienna, Austria, we captured the stable isotopic evolution during thunderstorms by sampling at intervals of 5 minutes or 0.2 mm of precipitation using an automated rain collection device (to date 640 samples from 43 precipitation events). We recorded meteorological information and drop size distribution (size vs. terminal velocity matrix) and other parameters related to precipitation intensity, such as the reflectivity aloft based on a vertical precipitation radar.

To distinguish the different source areas of storms, we applied backward trajectory analysis, aiming to partition Atlantic, Mediterranean, and continental origins. As a result, most of the rain amount in this period could be attributed to a handful of storm events. Our laboratory analytical approach was based on ultra-high precision replicated analysis of collected rain samples by Cavity-Ringdown Spectroscopy (CRDS). Triple oxygen isotopes (180/170/160) were analysed, though the precision/accuracy of  $\Delta$ 170 challenged the precision limits of CRDS technology.

First results demonstrate the complex progression of thunderstorms and rain events and indicate caution against explanations based on single predictors (e.g., temperature, precipitation amount). We observed that rain events with < 8 mm of precipitation tended to have a d-excess of < 10 % with a linear relationship with rain amount, whereby events > 8 mm tended to have a more typical deuterium excess between 10-15 %. Although these major rain events point at the same source region of south(east)ern Europe, such a generalized assessment overlooks the intra-rain-event dynamics, e.g., spanning a d-excess range of 16 % in total. Further work aims to disentangle the multifaceted nature of these storm events as a complex interaction between moisture sources, height of formation and sub-cloud alteration.

### The value of spatial representativeness for comparing satellite-retrieved and in-situ $\delta D$ measurements to isotope-enabled model simulations

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The abundancy of deuterium (denoted as  $\delta D$ ) in atmospheric water vapour can be studied using a variety of observational platforms that have a wide range of spatial and temporal resolutions. While satellite-retrieved products of  $\delta D$  in water vapour allow to study  $\delta D$  variability on spatial scales of several 1000km every 12-24h, the few available in-situ water vapour measurements of δD are at a much higher temporal resolution (seconds), and cover a more limited spatial extent (10s of km). To compare these different datasets to each other, and to model simulations, the dominant time and length scales of water vapour  $\delta D$  features in different parts of the atmosphere need to be considered. In this study, we asses the additional value of the newly developed retrieval of water isotopologues for the Sentinel 5P satellite, based on the University of Leicester Full Physics retrieval algorithm. The satellite dataset is available at a spatial resolution up to 7 km with a daily global coverage. Together with in-situ vertical profiles of  $\delta D$  from ultralight aircraft acquired during the L-WAIVE campaign in June 2019, the typical length scales of  $\delta D$  features on a synoptic time scale are determined, and compared to those obtained from model simulations with the isotope-enabled weather prediction model COSMOiso. The assessment of the spatial and temporal representativeness of these different datasets helps to guide towards an unbiased comparison of different datasets, and leads to more general recommendations for future comparison studies of in-situ measurement, satellite products, and model-simulated δD. Furthermore, the combination of in-situ measurements and COSMOiso simulations with satellite retrieved  $\delta D$  can help to better constrain vertical  $\delta D$  gradients and to understand the evolution of large scale  $\delta D$  patterns.

# Transient simulation of the past 2000 years with the isotope-enabled coupled model MPI-ESM-wiso

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The Common Era (CE, i.e. the past 2000 years) is among the periods selected by the Paleoclimate Modelling Intercomparison Project (PMIP) for transient experiments contributing to PMIP4. For PMIP4, novel estimates and updates of external forcing have been compiled (Jungclaus et al., GMD, 2017). In addition to the Tier-1 category simulation past1000 for the period 850 CE to 1849 CE, the Tier-3 past2k experiment covers the entire CE, extending the possibilities to evaluate the models' response to natural external forcing like volcanic activity. In this context, we present here a past2k experiment performed with the isotope-enabled version of the fully coupled model MPI-ESM, MPI-ESM-wiso, and potential paleoclimate applications.

As a first application, our simulation provides great opportunities to aid the interpretation of oxygen isotopic ratios (d18O) variations in response to volcanic eruptions. Indeed, since the volcanic eruptions do not affect only the temperature but also the water vapor distribution and its transport, the interpretation of d18O signals measured in natural archives can be complex. The analysis of our modeled isotope results during volcanic induced cooling period, like over the Northern Hemisphere in the mid 6th–7th century, and direct isotope model-data comparisons are then useful to better understand the impacts of volcanism on water isotopes and by extension on climate.

Our simulation products can also be used to reconstruct the climate variations of the last 2000 years, which is crucial to bring baseline information about Earth's natural climate variability in comparison of the current global warming. The PAGES 2k community made considerable efforts to produce such reconstructions based on different statistical technics using observations and/or model outputs. Thanks to our isotope-enabled model, we can use offline data assimilation directly on our isotope modeled results to reconstruct variations in climate variables over the past 2000 years. First results and issues related to this technic will be discussed.

# Variability in $\delta$ 2H and $\delta$ 18O of Soil Water and Its Linkage to Precipitation in An East Asian Monsoon Subtropical Forest Plantation

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Linkage between  $\delta$ 2H and  $\delta$ 18O of soil water and precipitation provides a way of understanding precipitation infiltration, residence time and soil water source. Soil water at 0-5, 15-20, and 40-45 cm depths and event-based precipitation were collected in a subtropical forest plantation. Correlations between  $\delta$ 18O of soil water and precipitation on the same day were used to determine critical threshold of precipitation infiltration. Residence time of precipitation before sampling. Soil water source was determined by the intersection points of Soil Water Evaporation Lines (SEL) and local meteoric water lines. The results showed precipitation > 5-6 mm could pass through canopy and litter, and infiltrate into soil. Residence times varied between a few days and several months, and increased with soil depth. The model-based approach for SEL estimation were more robust than the regression-based approach due to the inverse variability in  $\delta$ 2H and  $\delta$ 18O of soil water source and soil evaporative fractionation. Soil water at 0-5 cm depth originated mainly from precipitation in the current season, while those at 15-20 and 40-45 cm depths originated mainly from precipitation in the previous season.

#### Water stable isotope signature of precipitation from Switzerland related to moisture sources

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In Switzerland, air masses transporting moisture essentially originate from the Atlantic Ocean, the Mediterranean Sea and the Continental sector (East). Therefore, it is important to understand the regional link between the modern moisture source and the precipitation water isotopes in order to provide comprehensive records of past climate based on speleothem (cave carbonate) fluid inclusion waters, which are micrometric voids filled with water originating from past precipitation. We collected during three years water from daily precipitation events at Le Mormont MeteoSwiss station in northwestern Switzerland (Affolter et al., 2014; Affolter et al., 2020). Altogether, we performed 413 precipitation water isotope analyses on precipitation samples and determined  $\delta D$ .  $\delta$ 18O, deuterium excess (d) and 17Oexcess. In addition, we performed tritium (3H) analyses on 228 samples. We coupled these analyses with air parcel back-trajectories made for the Jura region performed at ETH Zurich. Results indicate that enhanced moisture contribution from the north Atlantic realm to winter precipitation brings more unpolluted marine moisture with close to Atlantic background 3H values. For water stable isotopes, results show that water isotopes have a different signature depending on the source. Furthermore, the secondary order parameters d and 17Oexcess also show a moisture source dependence with, in general, more positive values in both parameters for moisture coming from the Atlantic. lower values for the Mediterranean Sea and again lower for the Continental sector. A trend has also been observed on a global scale and suggests a potential dependence of the d/17Oexcess on the water phase, i.e. vapour, liquid or solid for reasons that still need to be investigated.

# Water stable isotopes in daily precipitation in Reykjavík during 2016-2021: Link to climate parameters and the isotope-enabled ECHAM5-wiso climate model

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While long-term monthly precipitation is available from Reykjavik, daily precipitation has not been sampled until now. A dataset covering almost continuous samples from rainy days for the last 5 years is now available. A large range is found in the daily isotopic values, where  $\delta$ 180 was found to range from -21.56 to +0.53‰,  $\delta$ D from -166.4 to +8.9‰ and the deuterium excess from -9.2 to +31.4‰. Deuterium excess shows significant anti-correlation with both temperature and specific humidity. A weaker positive correlation was observed between  $\delta$ 180 (and  $\delta$ D) and the weather parameters mentioned above. Relationship between the isotopic precipitation data and the North Atlantic Oscillation (NAO) suggests anti-correlation between  $\delta$ 180 (and  $\delta$ D) and the NAO index, especially during winter months, though statistically non-significant.

Moderate correlation was found between the observed isotope data and the isotope-enabled ECHAM5-wiso climate model for the period from 2016-2018.

#### Water vapor isotopic signature along the EAIIST traverse (East Antarctica Plateau)

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Stable water isotopes are a tracer of hydrological processes and a paleoclimate proxy from ice core records. The interpretation of the latter relies on fractionation processes throughout the hydrological cycle, from the evaporation over the ocean, during each precipitation event, and during post-deposition processes, in particular due to the exchanges between the snow and the moisture in the atmosphere. Thanks to new developments in infrared spectroscopy, it is now possible to monitor not only the snow isotopic composition but also the vapour continuously, and thus document exchanges between the snow and the vapour. On the East Antarctic Plateau, records of water vapour isotopic composition in Kohnen and Dome C during summer have revealed significant diurnal variability which can be used to address the exchange between surface snow and atmospheric water vapour as well as the stability of the atmospheric boundary layer.

In this study, we present the first vapour monitoring on a transect across East Antarctica for a period of 3 months from November 2019 to February 2020 during the traverse EAIIST, covering more than 3600 km. In parallel, we also monitored the vapour isotopic composition at two stations: Dumont D'Urville (DDU), at the starting and Dome C, half way through. Two automatic weathering stations were also installed at Paleo and Megadunes stations in a previously unexplored region of the East Antarctic plateau. Efforts on the calibration on each monitoring station, as well as cross-calibration of the different instruments offer a unique opportunity to compare both the spatial and temporal (diurnal variability or at the scale of several days) gradients of humidity, temperature and water vapour isotopic composition in East Antarctica during the summer season.

With the use of the Modele Atmospherique Régional (MAR), we compare the variability measured in water vapour, temperature and humidity with the different systems (fixed or mobile location). Although further comparisons with the surface snow isotopic composition are required to quantify the impact of the snow-atmosphere exchanges on the local surface mass balance, these three simultaneous measurements of the vapour isotopic composition show the potential of using water stables isotopes to evaluate hydrological processes in East Antarctica.

#### When microphysics matters for rain and clouds

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Many robust findings that rely on isotope ratio information have resulted from the assumption that rain and cloud water is near equilibrium when formed. This is an assumption which is at the basis of the Rayleigh distillation model. It is well known that rain at ground level does not follow this incloud behaviors due to isotopic exchange as raindrops fall though subsaturated environments. which is an out-of-equilibrium condition. At finer scales, thermodynamic disequilibrium in clouds is sustained by clouds-scale circulation and turbulence. Recent airborne measurements of isotope ratios in clouds provide a direct measure of disequilibrium between ambient water vapor and the condensate, and this can be leveraged to expose the underlying microphysical properties. In the case of snow formation, this is due to growth under supersaturated conditions, which give rise to substantial observable kinetic effects and has been known in principle to explain polar and alpine observations. For liquid clouds, the observed disequilibrium is unexpected, and is associated with active evaporation or growth of droplets - including in the case of mixed phase clouds. With a detailed accounting for microphysical exchanges, and gravitational selection due to drop size-dependent fall speeds, these basic properties are assessed. From a pragmatic standpoint, how microphysical can details scale up to cloud or precipitation event averages becomes critical. Do the microphysical details matter, or are simpler bulk assumptions adequate? A series of numerical experiments demonstrate the conditions under which either result is valid: the case of stratiform rain, and frontal rain is compared with the case of rain in the region of coldpool downdrafts. The results highlight that the sensitivity of isotope ratios to disequibrium effects enable measurements to a constraint cloud microphysics and rain processes that are otherwise difficult to capture in numerical models. We discuss the opportunities to target observations to expose these exchanges.