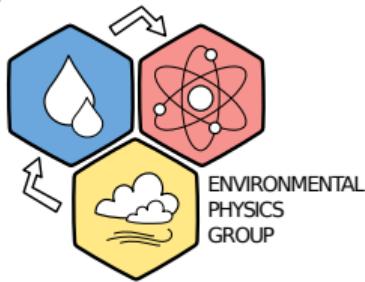


A particle-based microphysics study of isotope exchanges in a single-column rain-shaft model

Sylwester Arabas, Kazimierz Różański (& Sanket Bhiogate - PhD cand. recently joined)



AGH University in Krakow, Poland





■ IAEA/GNIP site in Kraków

The Global Network of Isotopes in Precipitation (GNIP) is a worldwide isotope monitoring network of hydrogen and oxygen isotopes in precipitation, initiated in 1960 by the International Atomic Energy Agency (IAEA) and the World Meteorological Organization (WMO), and operates in cooperation with numerous partner institutions in Member States.



- IAEA/GNIP site in Kraków
- 50-year precip isotopic data record

Global Network of Isotopes in Precipitation (GNIP)

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Access the Network



- ▶ IAEA/GNIP site in Kraków
- ▶ 50-year precip isotopic data record
- ▶ high-altitude lab (clouds in-situ)
@Kasprowy Wierch (6500 ft AMSL)



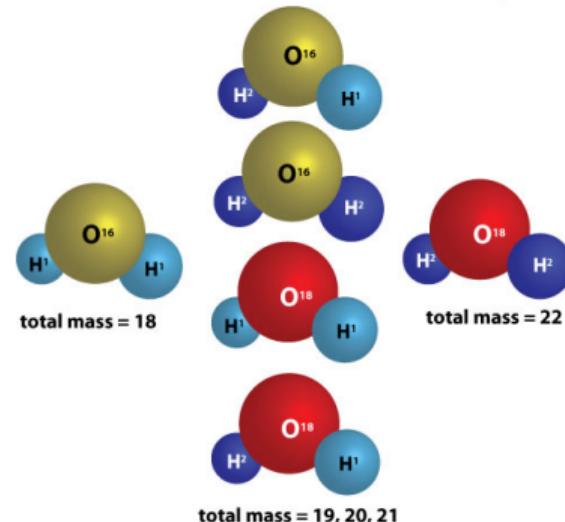
photo: naukaoklimacie.pl

clouds from a water isotopic point of view

- water isotopologues (stable): H_2O (99.7%), H_2^{18}O (0.2%), H_2^{17}O (0.04%), HDO (0.03%), ...

Oxygen and hydrogen isotopes in water

Light \longrightarrow Heavy

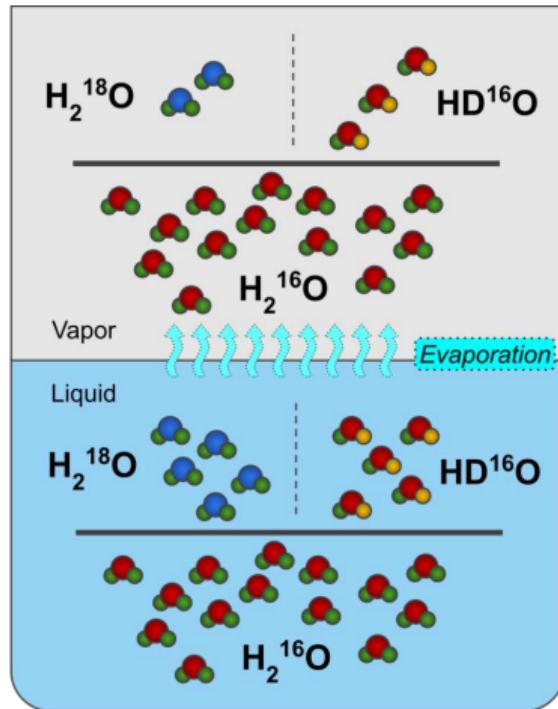


graphic: usgs.gov

$$M_d = 18.01528 \text{ g/mol}$$

clouds from a water isotopic point of view

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- condensation “favors” heavy over light isotopologues (evaporation vice versa)
 - equilibrium fractionation
 - more pronounced in colder temperatures
 - larger ($\times 8$) effect for H than O



graphic: scisnack.com

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- differences in diffusivity in air
 - ~~ non-equilibrium (kinetic) fractionation
 - ~~ applies to sub- and super-saturated conditions (+ liq/ice)
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$$\epsilon_{\text{kin}} \approx n \cdot \epsilon_{\text{diff}} \cdot (1 - RH)$$

ϵ_{kin} kinetic fractionation coeff.

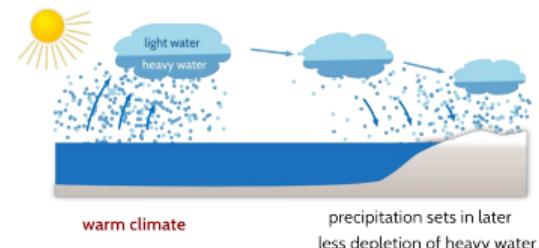
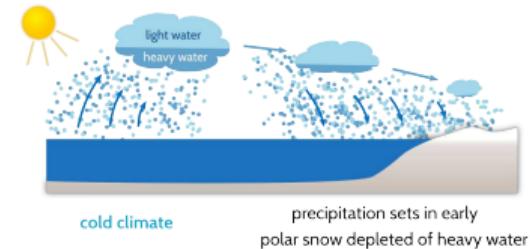
n turbulence parameter

ϵ_{diff} diffusive fractionation coeff.

RH rel. humidity

clouds from a water isotopic point of view

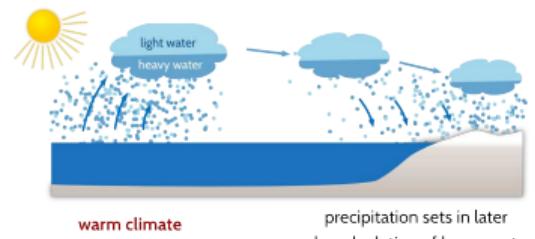
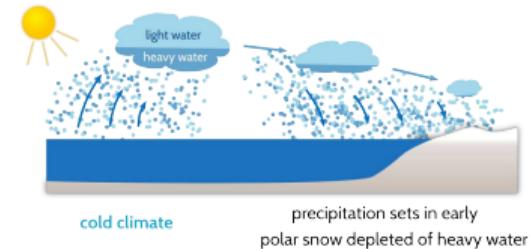
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- cloud μ -physics shapes isotopic composition of “meteoric water”
 - ~~ data for validation of μ -physical models!



graphic: physics-in-a-nutshell.com

clouds from a water isotopic point of view

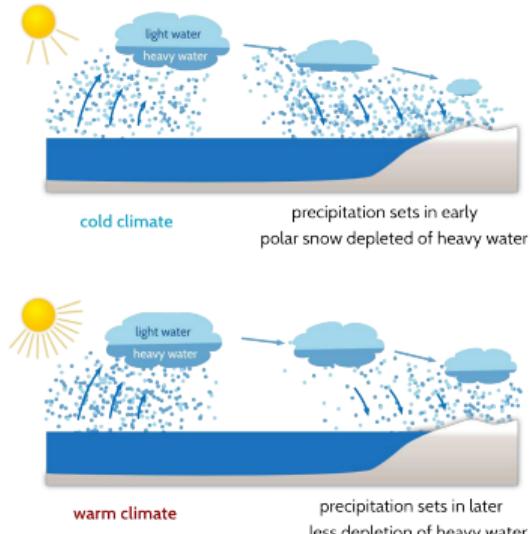
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 - ~~ data for validation of μ -physical models!
- ☒ freezing “freezes” the isotopic composition of water



graphic: physics-in-a-nutshell.com

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 - ~~ data for validation of μ -physical models!
- ☒ freezing “freezes” the isotopic composition of water
- ☒ isotope-aware μ -physics models in ice isotopic data analysis



graphic: physics-in-a-nutshell.com

let's equip a particle-based μ -physics package
with isotope fractionation model!

PySDM: open-source particle-based μ -physics modeling package

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PySDM 2.40

Released: Jan 22, 2024

`pip install PySDM` 

Pythonic particle-based (super-droplet) warm-rain/aqueous-chemistry cloud microphysics package with box, parcel & 1D/2D prescribed-flow examples in Python, Julia and Matlab

Navigation

-  Project description
-  Release history
-  Download files

Project description

PySDM


Maintained by  Open Hub  DOI: 10.21105/joss.03219 DOI: 10.5281/zenvnlo.10549422
EU Funding by FNP, PL Funding by NCN, US DOE Funding by ASR

License:  tests+artifacts+pypy:  build:  codecov: 62%
pypl package:  API docs: 

 [Homepage](#)

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- particle diffusional growth/evaporation (incl. CCN activation)

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Project description

PySDM

PySDM is a Pythonic particle-based (super-droplet) warm-rain/aqueous-chemistry cloud microphysics package. It includes models for particle diffusion, evaporation, and activation, as well as collisional growth and breakup (Monte-Carlo, SDM). The package supports various environments (Python 3, LLVM, Numba, CUDA, ThreadSafe, Linux, macOS, Windows, jupyter), and is maintained by the PySDM team. It has been released on Open Hub, has a DOI of 10.5281/zenodo.10549422, and is funded by EU, FNP, NCN, and US DOE. The code is licensed under GPL v3 and is available on GitHub. PySDM has a test coverage of 82% and is published on PyPI with version 2.40.

- particle diffusional growth/evaporation (incl. CCN activation)
- collisional growth and breakup (Monte-Carlo, SDM)

PySDM: open-source particle-based μ -physics modeling package



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PySDM is maintained by [jess](#) and was last updated on Jan 22, 2024. It has a DOI of [10.5281/zenodo.10549422](#). It is funded by FNP, NCN, and US DOE.

PySDM is licensed under [GPL v3](#). It has a test coverage of 62% and is built using [pyproject.toml](#).

- particle diffusional growth/evaporation (incl. CCN activation)
- collisional growth and breakup (Monte-Carlo, SDM)
- aqueous-phase oxidation of SO₂ by H₂O₂ and O₃

PySDM: open-source particle-based μ -physics modeling package

The screenshot shows the GitHub project page for PySDM 2.40. The top navigation bar includes links for Help, Sponsors, Log in, and Register. A search bar is present. The main content area features a large green "Latest version" button. Below it, the release date is listed as "Released: Jan 22, 2024". A "pip install PySDM" button is shown. The project description states: "Pythonic particle-based (super-droplet) warm-rain/aqueous-chemistry cloud microphysics package with box, parcel & 1D/2D prescribed-flow examples in Python, Julia and Matlab". The left sidebar has sections for Navigation (Project description, Release history, Download files), Project links (Homepage), and a detailed Project description for PySDM.

- ❖ particle diffusional growth/evaporation (incl. CCN activation)
- ❖ collisional growth and breakup (Monte-Carlo, SDM)
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- ❖ immersion freezing (Monte-Carlo, ABIFM)

PySDM: open-source particle-based μ -physics modeling package

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- ❖ features 0D, 1D and 2D example simulation setups

PySDM: open-source particle-based μ -physics modeling package

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PySDM

Python 3 LLVM Numba CUDA Threadsafe Linux macOS Windows Jupyter Maintained by Open Hub PySDM DOI 10.21105/joss.03219 DOI 10.5281/zenodo.1054942 EU Funding by FNP PL Funding by NCN US DOE Funding by ASR License GPL v3 tests+artifacts+pypy packaging build packaging codecov 62% pypl package 240 API docs pypi

- particle diffusional growth/evaporation (incl. CCN activation)
- collisional growth and breakup (Monte-Carlo, SDM)
- aqueous-phase oxidation of SO₂ by H₂O₂ and O₃
- immersion freezing (Monte-Carlo, ABIFM)
- features 0D, 1D and 2D example simulation setups
- 100% Python code (LLVM via Numba + GPU)

PySDM: Jupyter notebooks reproducing results from literature

pypi.org/p/PySDM-examples

literature reference	cond / evap	coalescence	isotopes	breakup	transport	chemistry	freezing	keywords
formulae-only								
Pierchala et al. 2022			x					#lab-experiment
OD box environment								
Berry 1967		x						#kernels
Shima et al. 2009		x						#analytic-solution
Alpert & Knopf 2016						x		#ABIFM
Bieli et al. 2022		x	x					#ML
de Jong et al. 2023		x	x					#analytic-solution
OD parcel environment								
Rozanski & Sonntag 1982	x		x					#iterative-parcel
Abdul-Razzak & Ghan 2000	x							#parameterisation
Kreidenweis et al. 2003	x				x			#Hoppel-gap
Arabas and Shima 2017	x					x		#timescales
Jaruga & Pawlowska 2018	x				x			#Hoppel-gap
Yang et al. 2018	x						x	#ripening
Lowe et al. 2019	x							#surfactants
Grabowski and Pawlowska 2023	x							#ripening
1D single-column kinematic env.								
Shipway & Hill 2012	x	x			x			#KiD
deJong et al. 2023 (figures 6-8)	x	x		x	x			#KiD
2D prescribed-flow environment								
Arabas et al. 2015	x	x			x			#GUI
Arabas et al. 2023 (figure 11)	x	x			x		x	#Paraview

^alaunch-in-the-cloud URL: https://mybinder.org/v2/gh/open-atmos/PySDM.git/main?urlpath=lab/tree/examples/PySDM_examples/Pierchala_et_al_2022

new PySDM “example” (incl. numerous automated tests) based on:

doi:10.1016/j.gca.2022.01.020

Geochimica et Cosmochimica Acta 322 (2022) 244–259

www.elsevier.com/locate/gca

Quantification the diffusion-induced fractionation of $^1\text{H}_2^{17}\text{O}$ isotopologue in air accompanying the process of water evaporation

Anna Pierchala ^{*}, Kazimierz Rozanski, Marek Dulinski, Zbigniew Gorczyca

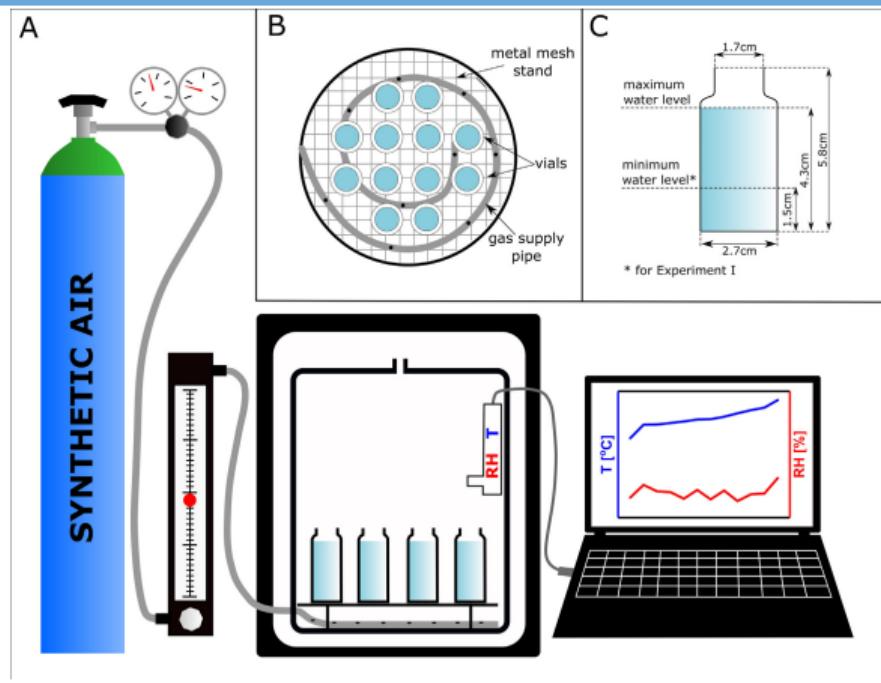
AGH University of Science and Technology, Faculty of Physics and Applied Computer Science, al. Mickiewicza 30, 30-059 Krakow, Poland

Received 25 February 2021; accepted in revised form 15 January 2022; Available online 24 January 2022

Pierchala et al. '22 – triple isotope analysis, kinetic fractionation^a

^alaunch-in-the-cloud URL: https://mybinder.org/v2/gh/open-atmos/PySDM.git/main?urlpath=lab/tree/examples/PySDM_examples/Pierchala_et_al_2022

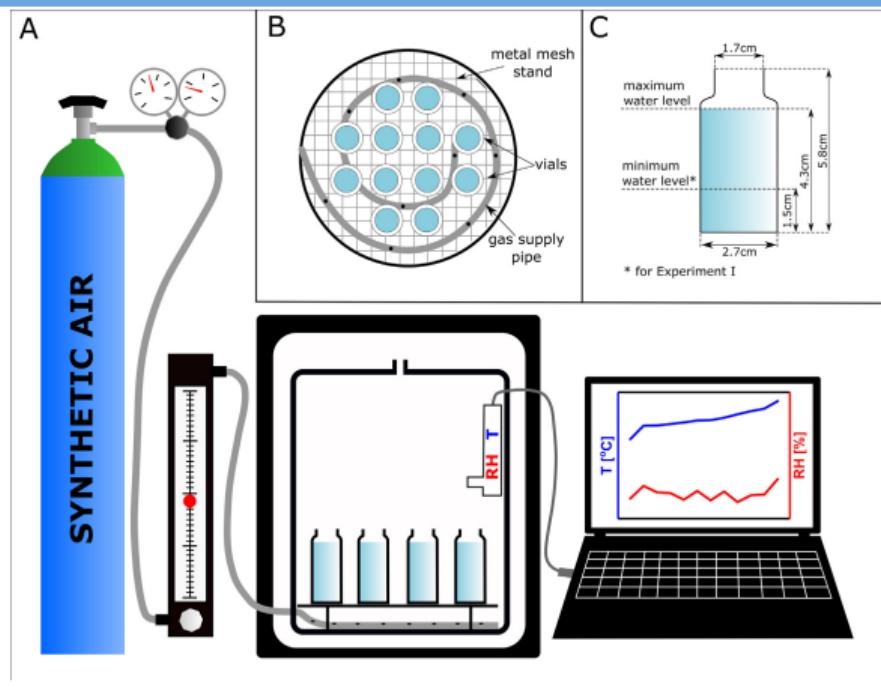
Fig. 1 (paper): lab experiment setup



Pierchala et al. '22 – triple isotope analysis, kinetic fractionation^a

^alaunch-in-the-cloud URL: https://mybinder.org/v2/gh/open-atmos/PySDM.git/main?urlpath=lab/tree/examples/PySDM_examples/Pierchala_et_al_2022

Fig. 1 (paper): lab experiment setup

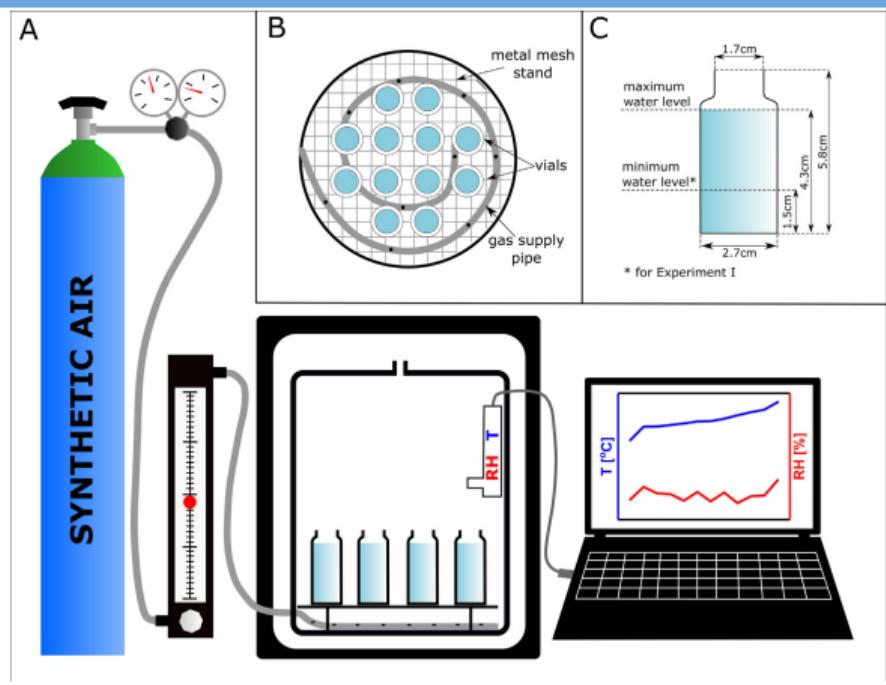


- fractionation upon evaporation (incl. kinetic effects)

Pierchala et al. '22 – triple isotope analysis, kinetic fractionation^a

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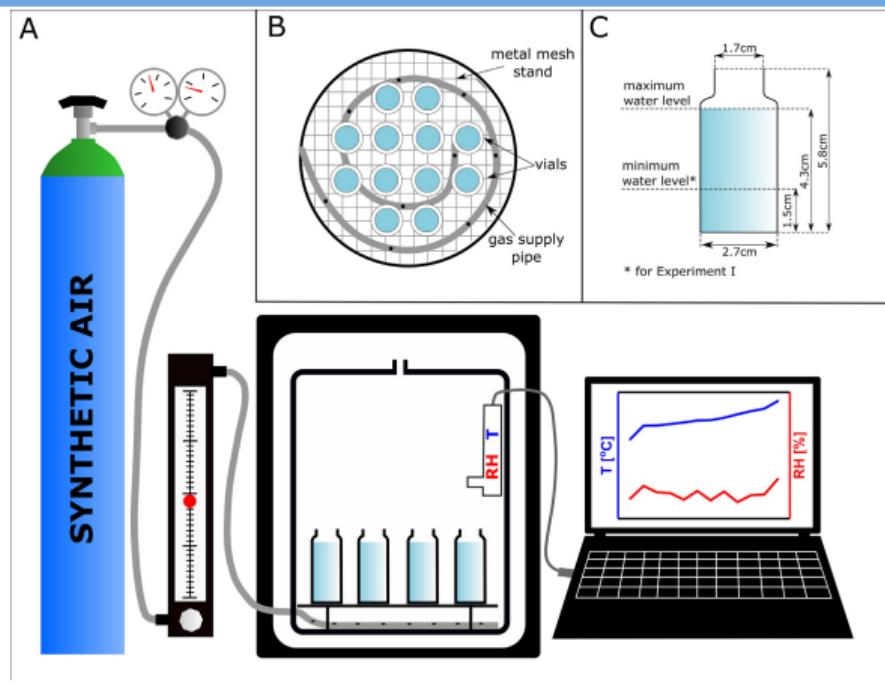


- fractionation upon evaporation (incl. kinetic effects)
- multi-day experiments (up to two weeks)

Pierchala et al. '22 – triple isotope analysis, kinetic fractionation^a

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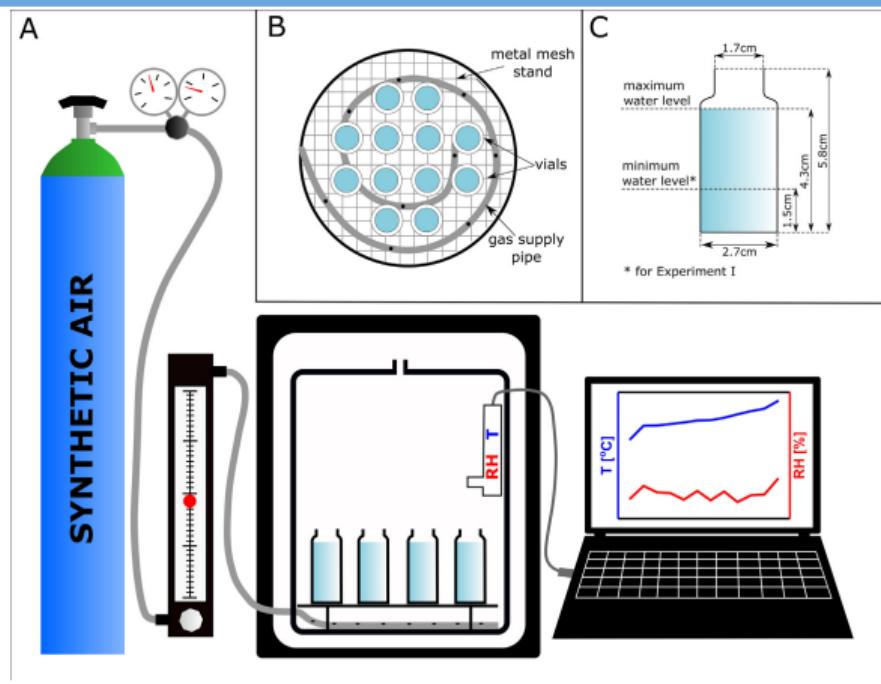


- fractionation upon evaporation (incl. kinetic effects)
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- Picarro L2140-i cavity ring-down laser spectrometer (D , ^{18}O , ^{17}O) (probing vaporized water)

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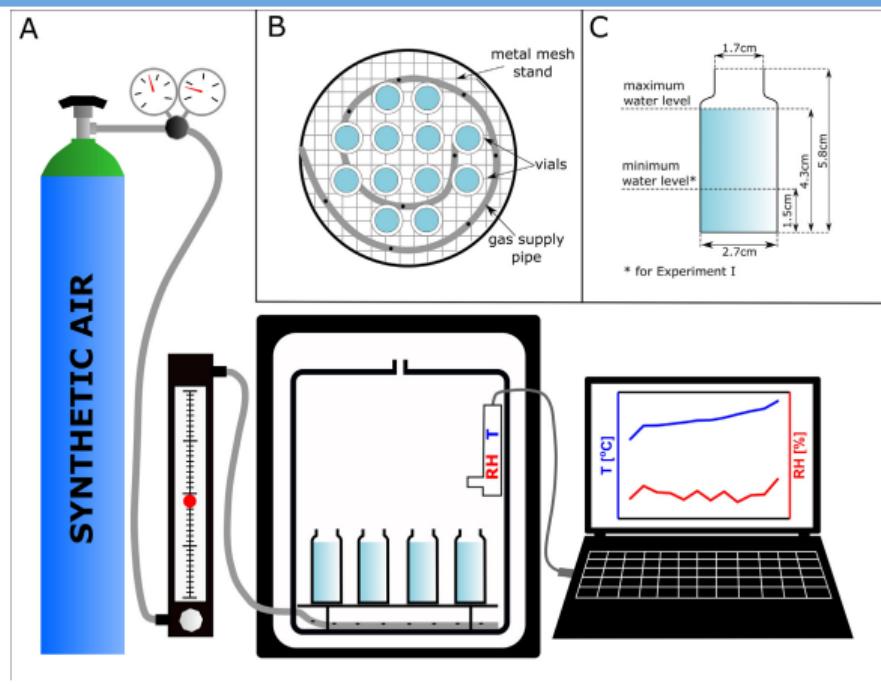


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Pierchala et al. '22 – triple isotope analysis, kinetic fractionation^a

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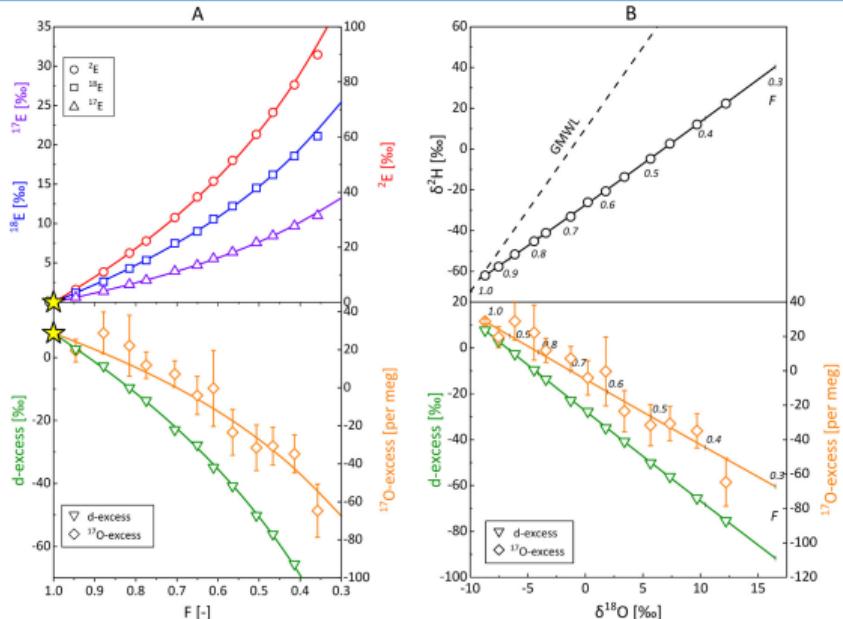


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- ❖ Picarro L2140-i cavity ring-down laser spectrometer (D , ^{18}O , ^{17}O) (probing vaporized water)
- ❖ constant T/RH, variable T or variable RH setups
- ❖ analysis against Rayleigh distillation + Craig-Gordon RH-dependence

Pierchala et al. '22 – triple isotope analysis, kinetic fractionation^a

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Fig. 3 (paper): measurements + model



$$E = \frac{[\text{heavy iso.}]}{[\text{light iso.}]} / \frac{[\text{heavy iso.}]}{[\text{light iso.}]} \Big|_{t=0} - 1$$

$$\delta = \frac{[\text{heavy iso.}]}{[\text{light iso.}]} / \frac{[\text{heavy iso.}]}{[\text{light iso.}]} \Big|_{\text{VSMOW}} - 1$$

F: fraction of water remaining

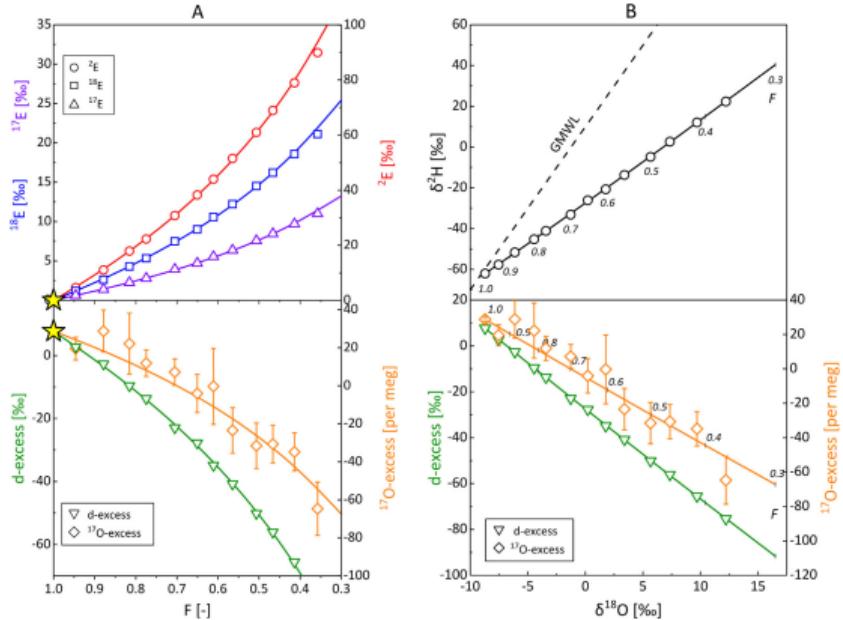
d-excess: $\delta^{2\text{H}} - 8 \cdot \delta^{18\text{O}}$

$^{17}\text{O}\text{-excess}: \ln(\delta^{17\text{O}} + 1) - 0.528 \cdot \ln(\delta^{18\text{O}} + 1)$

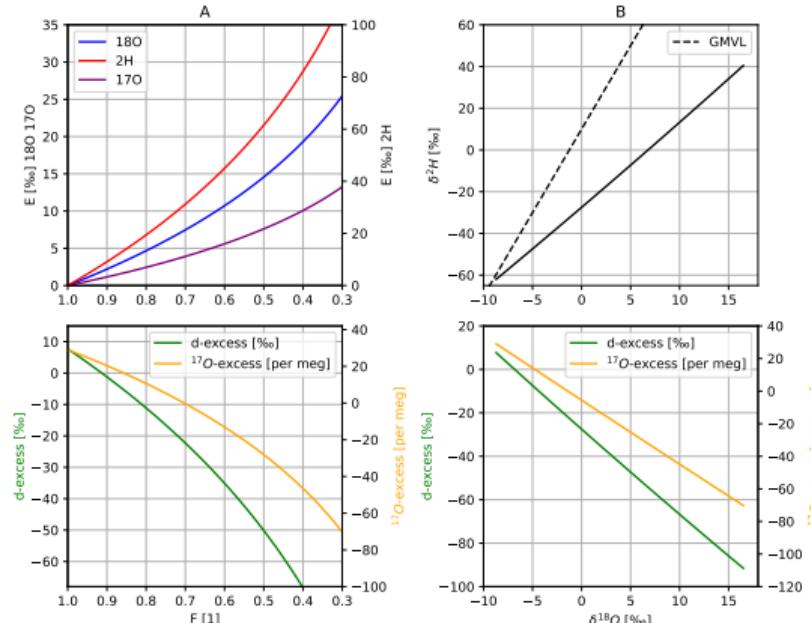
Pierchala et al. '22 – triple isotope analysis, kinetic fractionation^a

^alaunch-in-the-cloud URL: https://mybinder.org/v2/gh/open-atmos/PySDM.git/main?urlpath=lab/tree/examples/PySDM_examples/Pierchala_et_al_2022

Fig. 3 (paper): measurements + model



PySDM: theoretical curves



$$E = \left[\frac{\text{heavy iso.}}{\text{light iso.}} \right] / \left[\frac{\text{heavy iso.}}{\text{light iso.}} \right]_{t=0} - 1$$

$$\delta = \left[\frac{\text{heavy iso.}}{\text{light iso.}} \right] / \left[\frac{\text{heavy iso.}}{\text{light iso.}} \right]_{\text{VSMOW}} - 1$$

F: fraction of water remaining

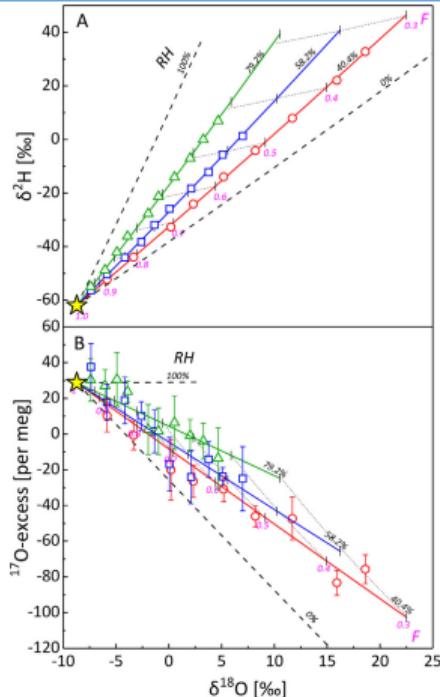
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$$^{17}\text{O}-\text{excess: } \ln(\delta^{17}\text{O} + 1) - 0.528 \cdot \ln(\delta^{18}\text{O} + 1)$$

Pierchala et al. '22 – triple isotope analysis, kinetic fractionation^a

^alaunch-in-the-cloud URL: https://mybinder.org/v2/gh/open-atmos/PySDM.git/main?urlpath=lab/tree/examples/PySDM_examples/Pierchala_et_al_2022

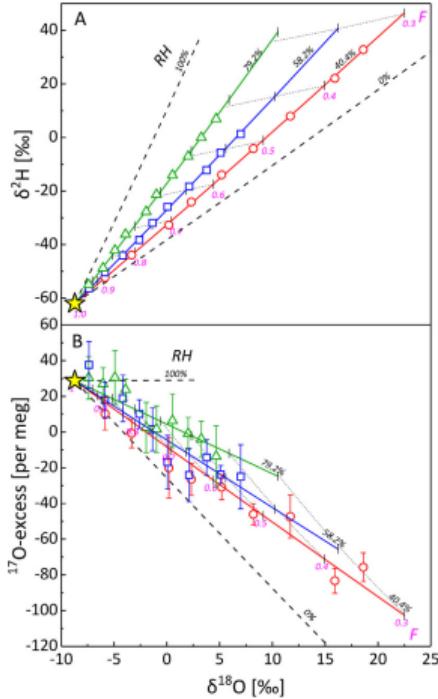
Fig. 4 (paper): RH varied



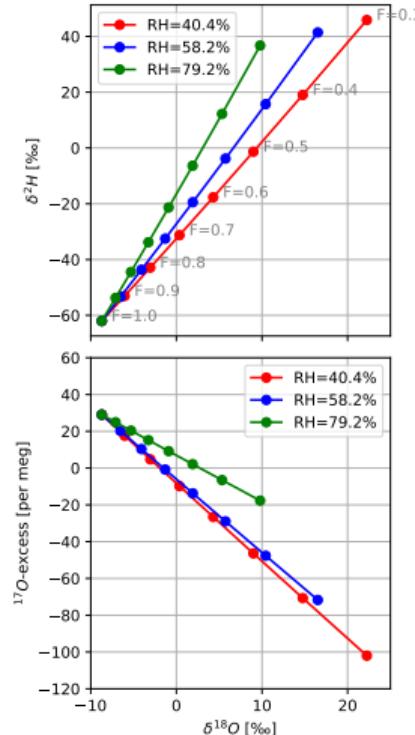
Pierchala et al. '22 – triple isotope analysis, kinetic fractionation^a

^alaunch-in-the-cloud URL: https://mybinder.org/v2/gh/open-atmos/PySDM.git/main?urlpath=lab/tree/examples/PySDM_examples/Pierchala_et_al_2022

Fig. 4 (paper): RH varied



PySDM: model curves



Rozanski & Sonntag '82 – multibox cloud/precip column model^a

^alaunch-in-the-cloud URL: https://mybinder.org/v2/gh/slayoo/PySDM.git/isotopes_rozanski_and_sonntag_example?urlpath=lab/tree/examples/PySDM_examples

new PySDM “example” (work in progress):

doi:10.3402/tellusa.v34i2.10795

Tellus (1982), 34, 135–141

Vertical distribution of deuterium in atmospheric water vapour

By K. ROZANSKI¹ and C. SONNTAG, *Institute of Environmental Physics, University of Heidelberg,
Im Neuenheimer Feld 366, D-6900 Heidelberg, F. R. Germany*

(Manuscript received September 26, 1980; in final form May 12, 1981)

Rozanski & Sonntag '82 – multibox cloud/precip column model^a

^alaunch-in-the-cloud URL: https://mybinder.org/v2/gh/slayoo/PySDM.git/isotopes_rozanski_and_sonntag_example?urlpath=lab/tree/examples/PySDM_examples

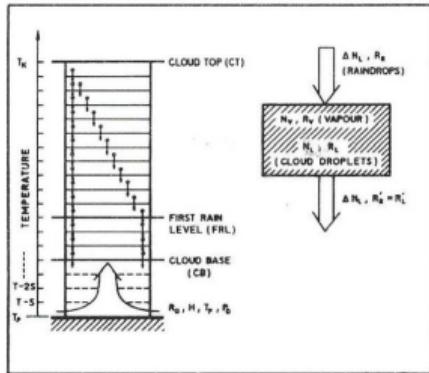
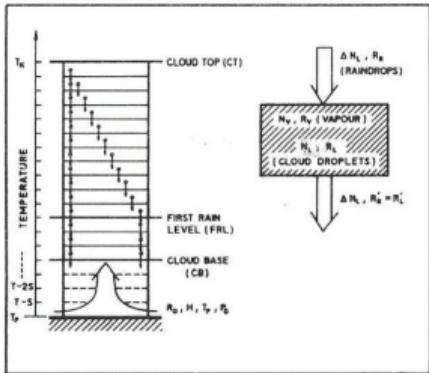


Fig. 3. Schematic diagram of the multibox cloud model.
Input data: initial temperature, T_p ; final temperature, T_k ; initial pressure, P_0 ; relative humidity, H ; initial isotopic composition of water vapour, R_0 ; cloud water mixing ratio, N_L ; temperature step, S ; isotope exchange factor, K .

Tellus 34 (1982), 2

Rozanski & Sonntag '82 – multibox cloud/precip column model^a

^alaunch-in-the-cloud URL: https://mybinder.org/v2/gh/slayoo/PySDM.git/isotopes_rozanski_and_sonntag_example?urlpath=lab/tree/examples/PySDM_examples



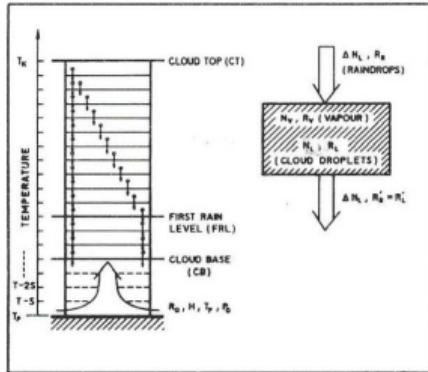
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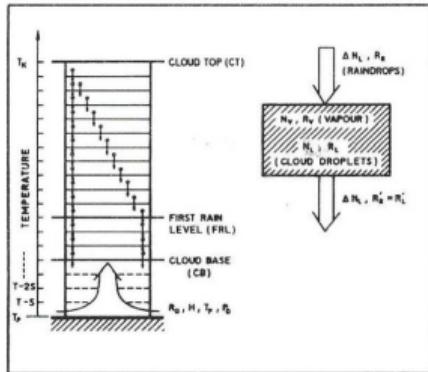


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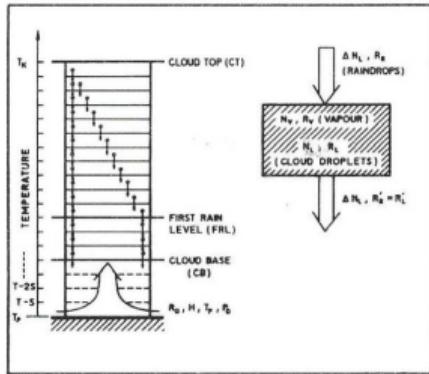


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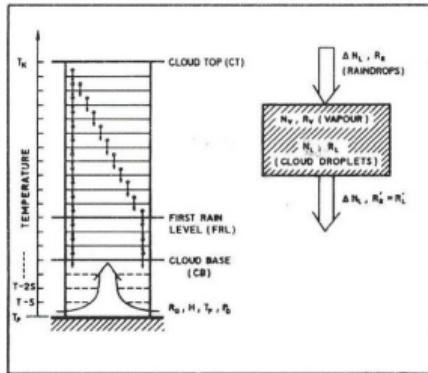


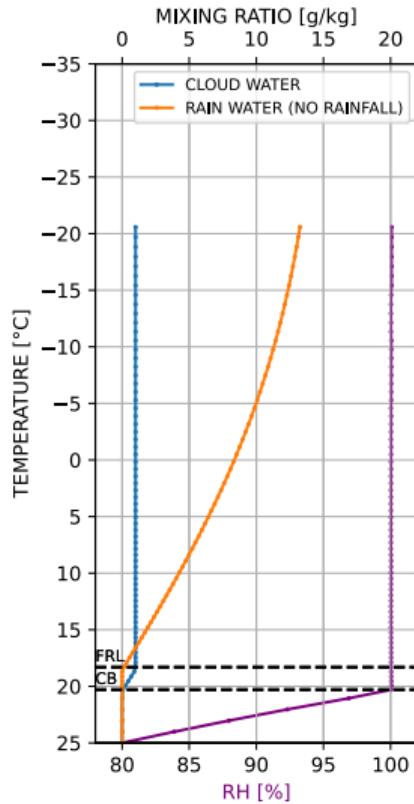
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- ▶ minimal model for capturing isotope exchange between precip, ambient vapor and cloud water (↔ hypothesis explaining observed steep $\delta^2\text{H}$ profile gradients beyond condensation-only effects)

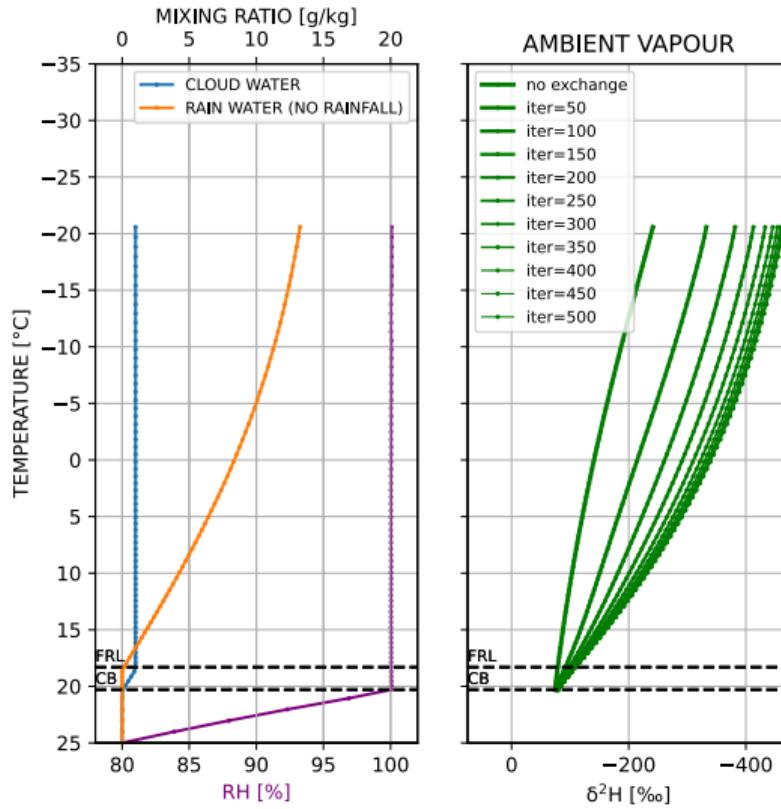
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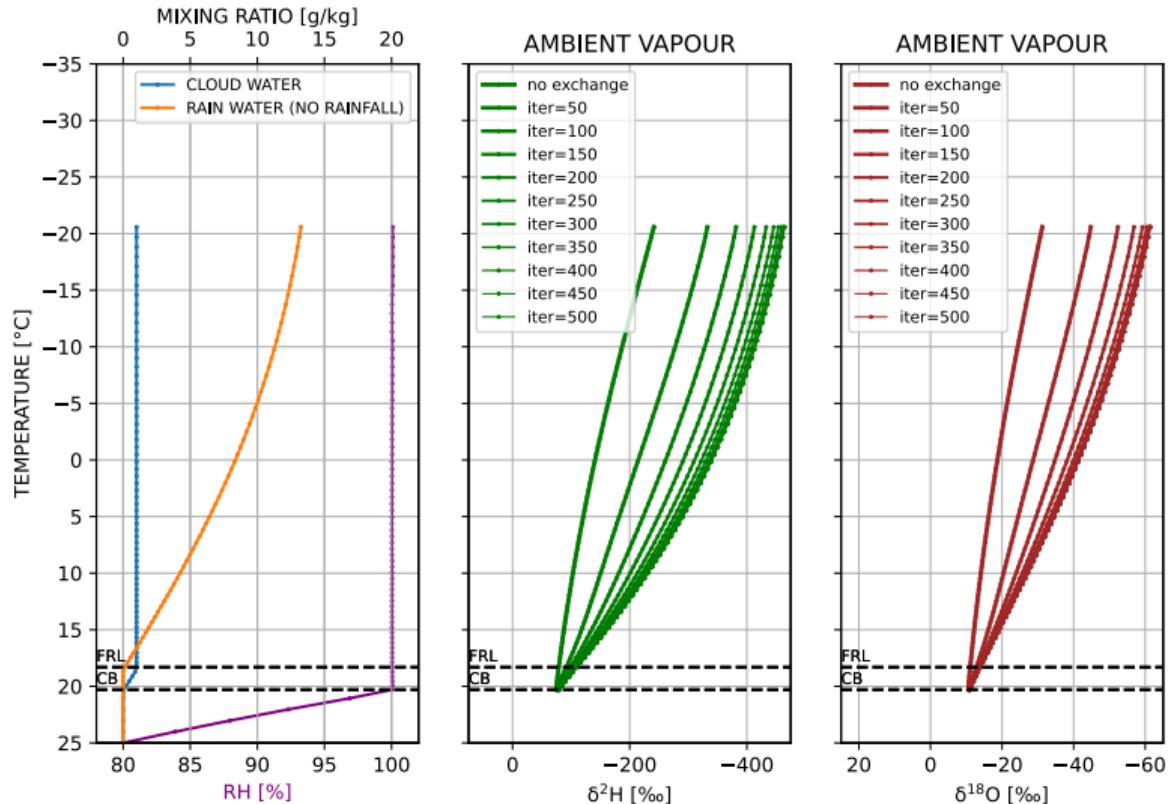
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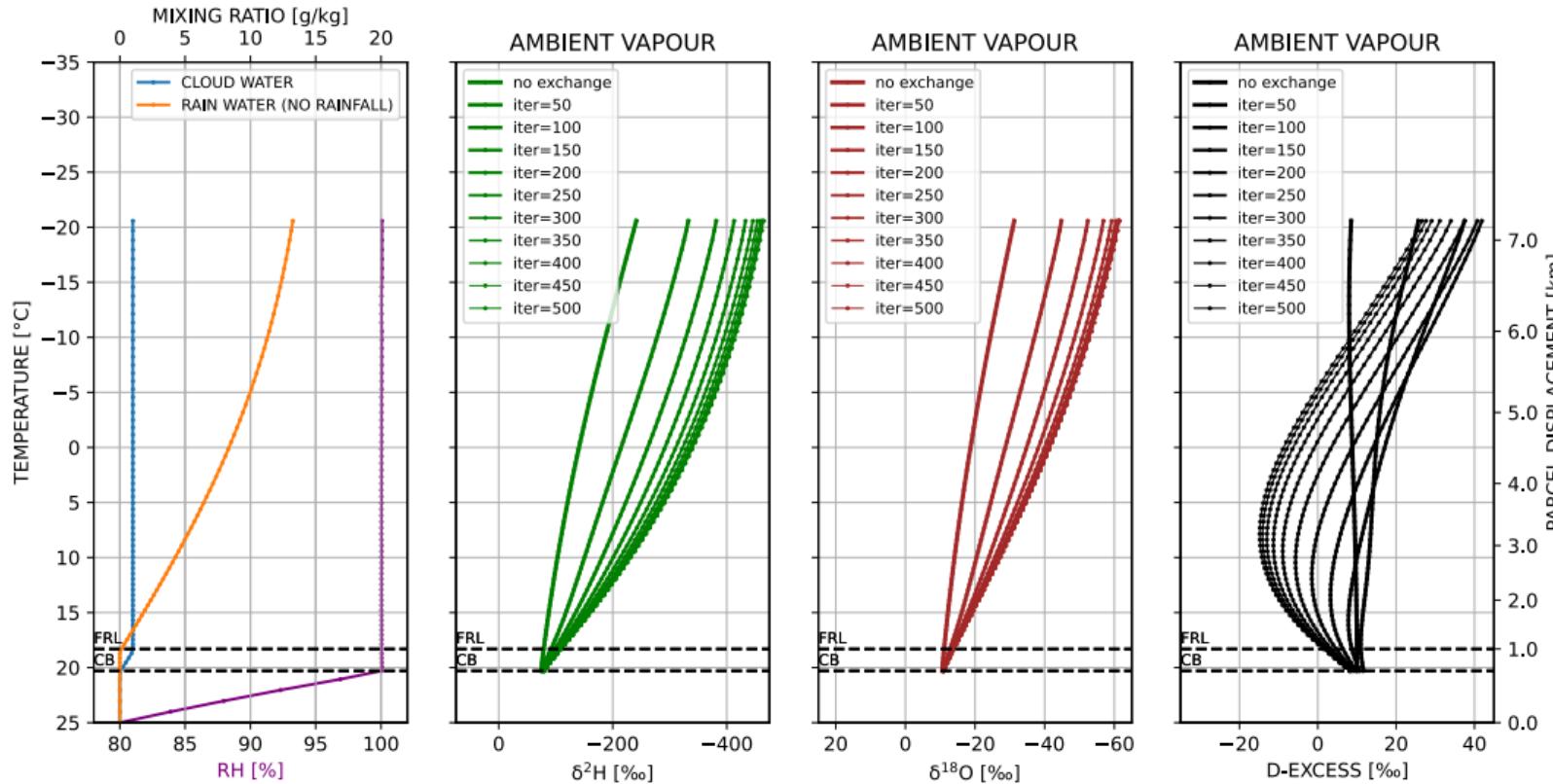
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implemented features (incl. tests against lab and model literature data):

- base SD attributes: #moles of heavy isotopologue

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- ☒ ice-phase processes

Thank you for your attention!

(sylwester.arabas@agh.edu.pl)



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