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

AGH University in Krakow, Poland

104th AMS Annual Meeting | Baltimore, MD | Jan 29 2024

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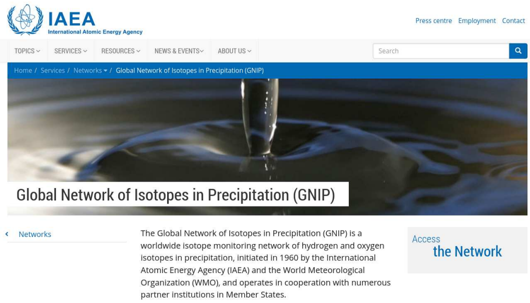
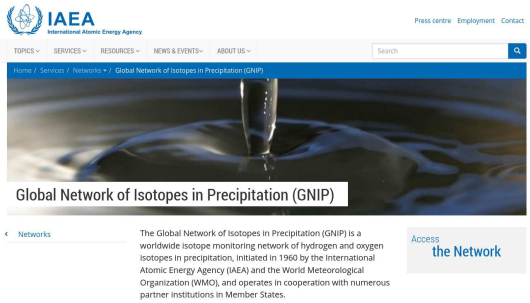
PHYSICS
GROUP



- IAEA/GNIP site in Kraków



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

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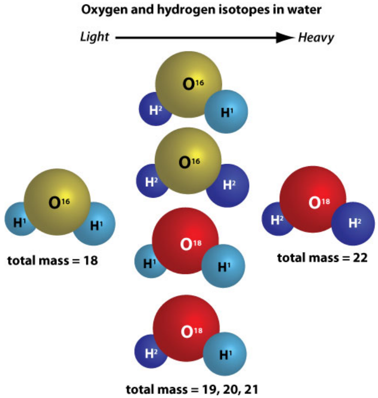
- IAEA/GNIP site in Kraków
- 50-year precip isotopic data record
- high-altitude lab (clouds in-situ) @Kasprowy Wierch (6500 ft AMSL)

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%), ...



graphic: usgs.gov

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

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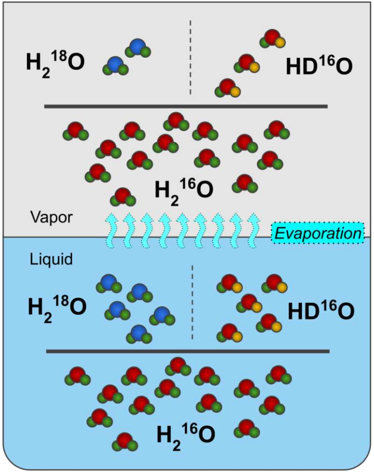
- condensation "favors" heavy over light isotopologues (evaporation vice versa)
  $\rightsquigarrow$ equilibrium fractionation
  $\rightsquigarrow$ more pronounced in colder temperatures
  $\rightsquigarrow$ larger ($\times 8$) effect for H than O



graphic: scisnack.com

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- differences in diffusivity in air
  $\rightsquigarrow$ non-equilibrium (kinetic) fractionation
  $\rightsquigarrow$ applies to sub- and super-saturated conditions (+ liq/ice)
  $\rightsquigarrow$ more pronounced for O than H

$$\epsilon_{\text{kin}} \approx n \cdot \epsilon_{\text{diff}} \cdot (1 - RH)$$

ϵ_{kin}	kinetic fractionation coeff.
n	turbulence parameter
ϵ_{diff}	diffusive fractionation coeff.
RH	rel. humidity

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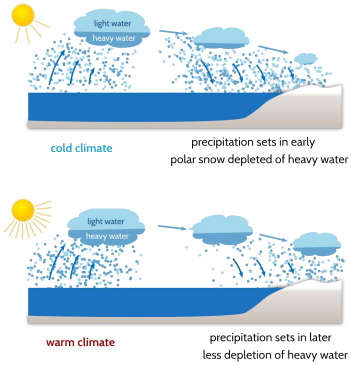
  ⇝ data for validation of μ-physical models!



graphic: physics-in-a-nutshell.com

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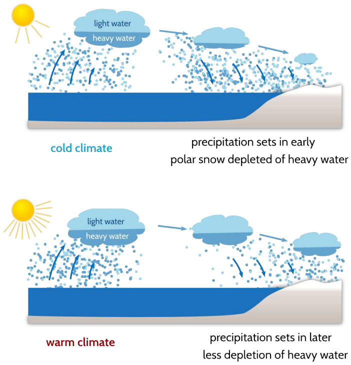

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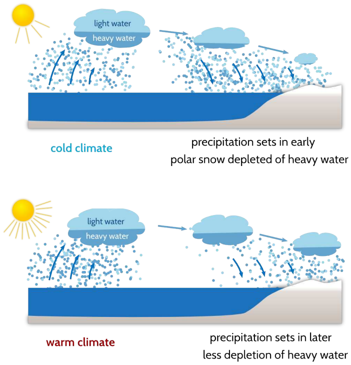
- isotope-aware μ-physics models in ice isotopic data analysis



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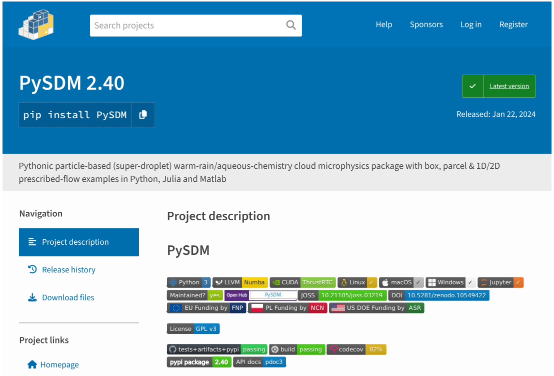
let's equip a particle-based μ-physics package
with isotope fractionation model!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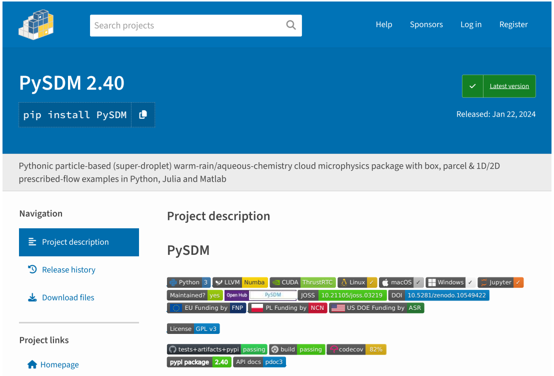
PySDM 2.40
pip install PySDM
Latest version
Released: Jan 22, 2024
Pythonic particle-based (super-droplet) warm-rain/aqueous-chemistry cloud microphysics package with box, parcel & 1D/2D prescribed-flow examples in Python, Julia and Matlab
Navigation
Project description
Release history
Download files
Project links
Homepage
Project description
PySDM
Python 3
LLVM Numba
CUDA ThrustRTC
Linux ✓
macOS ✓
Windows ✓
Jupyter ✓
Maintained? yes
Open Hub PySDM
JOSS 10.21105/joss.03219
DOI 10.5281/zenodo.10549422
EU Funding by FNP
PL Funding by NCN
US DOE Funding by ASR
License GPL v3
tests+artifacts+pypi passing
build passing
codecov 82%
pypi package 2.40
API docs pdoc3

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



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

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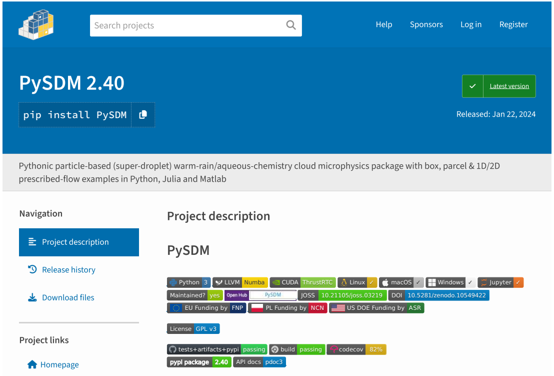

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- collisional growth and breakup (Monte-Carlo, SDM)

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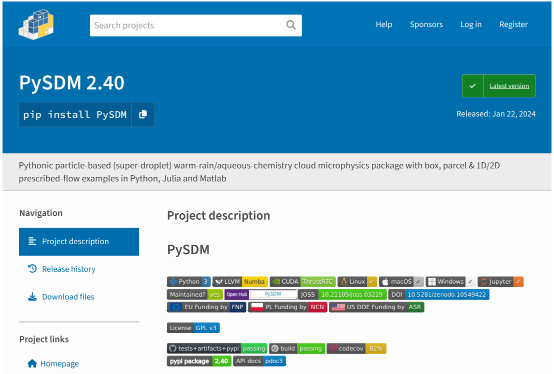

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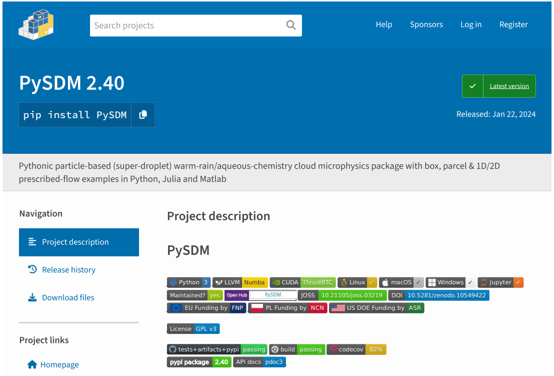

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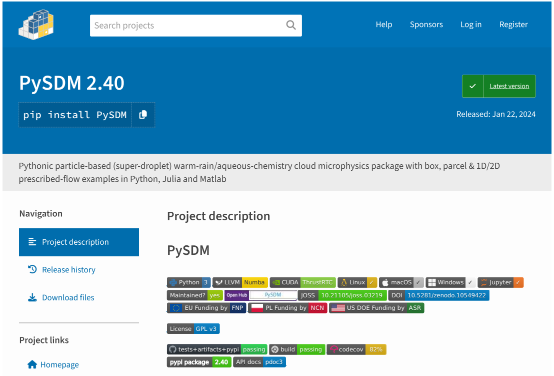

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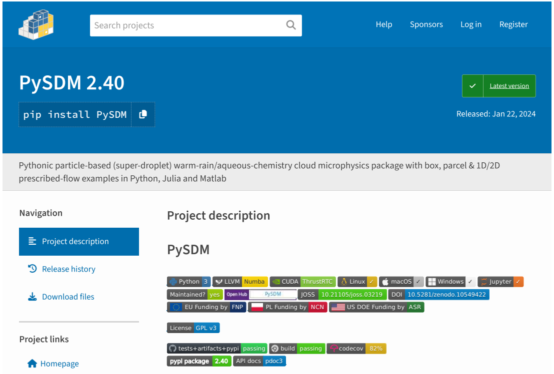

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- aqueous-phase oxidation of SO_2 by H_2O_2 and O_3
- immersion freezing (Monte-Carlo, ABIFM)
- features 0D, 1D and 2D example simulation setups
- 100% Python code (LLVM via Numba + GPU)

PySDM: Jupyer 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			×					#lab-experiment
0D box environment								
Berry 1967		×						#kernels
Shima et al. 2009		×						#analytic-solution
Alpert & Knopf 2016							×	#ABIFM
Bieli et al. 2022		×		×				#ML
de Jong et al. 2023		×		×				#analytic-solution
0D parcel environment								
Rozanski & Sonntag 1982	×		×					#iterative-parcel
Abdul-Razzak & Ghan 2000	×							#parameterisation
Kreidenweis et al. 2003	×					×		#Hoppel-gap
Arabas and Shima 2017	×							#timescales
Jaruga & Pawlowska 2018	×					×		#Hoppel-gap
Yang et al. 2018	×							#ripening
Lowe et al. 2019	×							#surfactants
Grabowski and Pawlowska 2023	×							#ripening
1D single-column kinematic env.								
Shipway & Hill 2012	×	×			×			#KiD
deJong et al. 2023 (figures 6-8)	×	×		×	×			#KiD
2D prescribed-flow environment								
Arabas et al. 2015	×	×			×			#GUI
Arabas et al. 2023 (figure 11)	×	×			×		×	#Paraview

[a]launch-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 $^{1}H_2^{17}O$ isotopologue in air accompanying the process of water evaporation

Anna Pierchala *, Kazimierz Rozanski, Marek Dulinski, Zbigniew Gorczyca

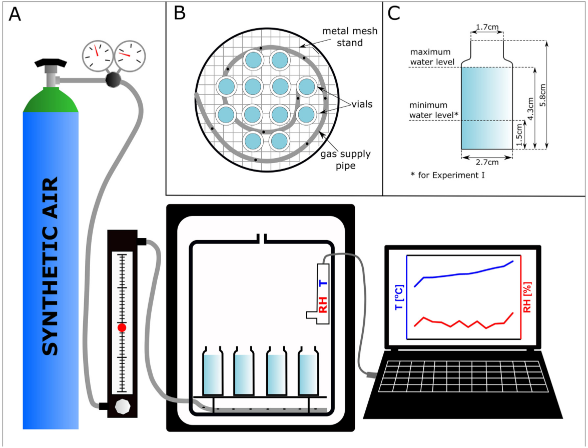
AGH University of Science and Technology, Faculty of Physics and Applied Computer Science, al. Mickiewicza 30, 30-059 Krakow, Poland

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]

[a]launch-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]

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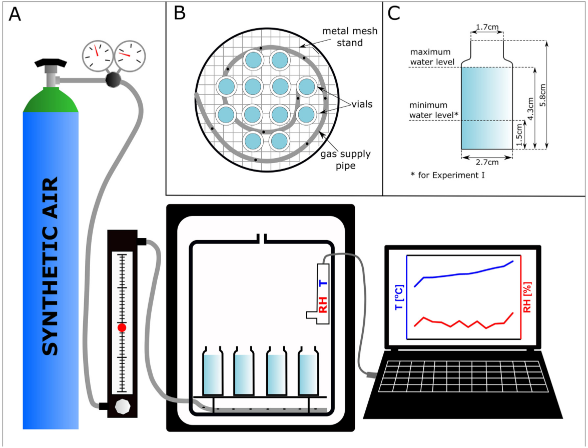

- fractionation upon evaporation (incl. kinetic effects)

Pierchala et al. ’22 – triple isotope analysis, kinetic fractionation[a]

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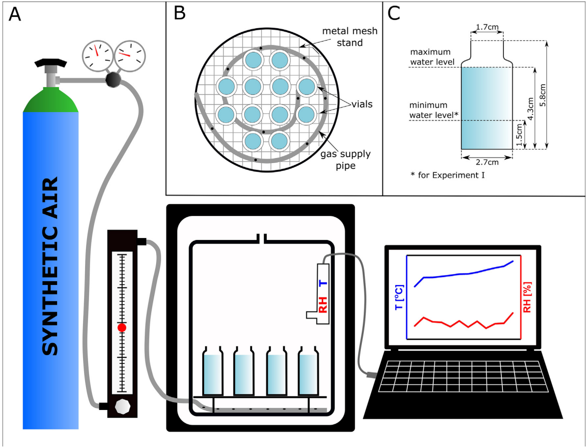

- fractionation upon evaporation (incl. kinetic effects)
- multi-day experiments (up to two weeks)

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

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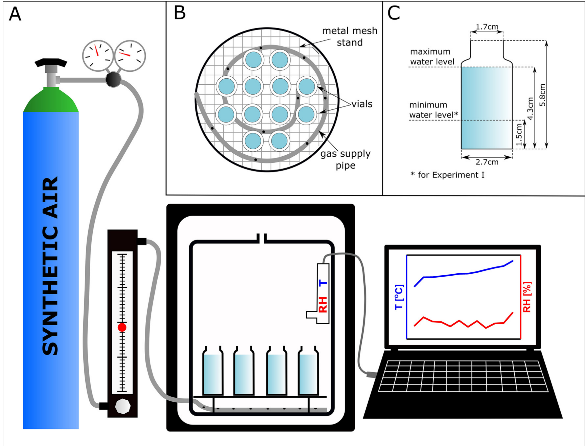

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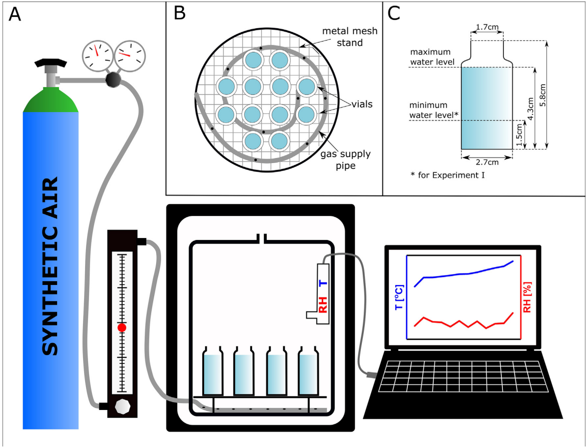

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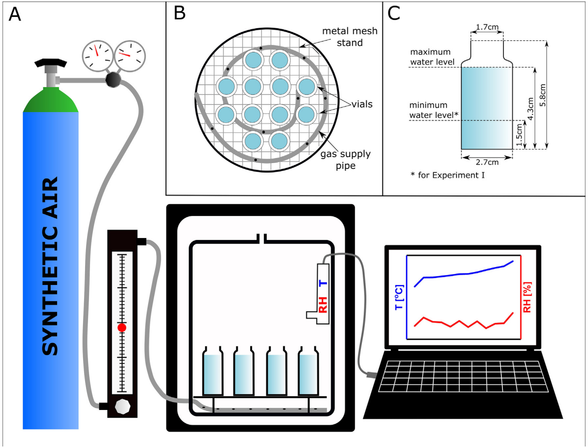

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- constant T/RH, variable T or variable RH setups
- analysis against Rayleigh distillation + Craig-Gordon RH-dependence

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

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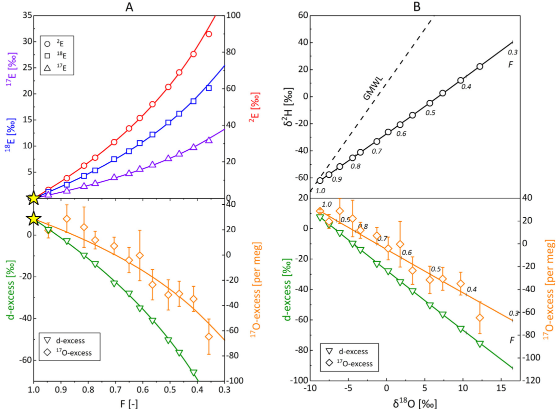
Fig. 3 (paper): measurements + model



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

F: fraction of water remaining

d-excess: $\delta^2 H - 8 \cdot \delta^{18} O$ $\quad$ ^{17}O-excess: $\ln(\delta^{17}O + 1) - 0.528 \cdot \ln(\delta^{18}O + 1)$

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

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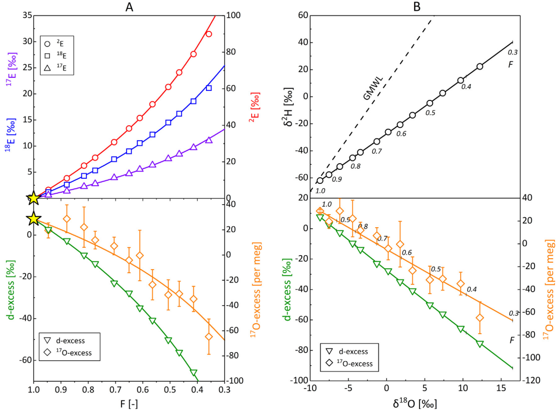

PySDM: theoretical curves

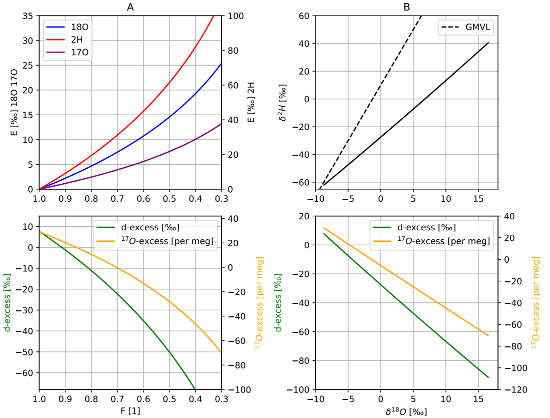

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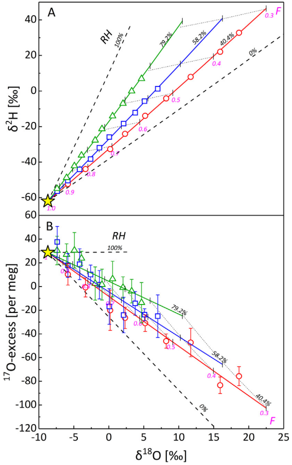
Fig. 4 (paper): RH varied



Pierchala et al. ’22 – triple isotope analysis, kinetic fractionation[a]

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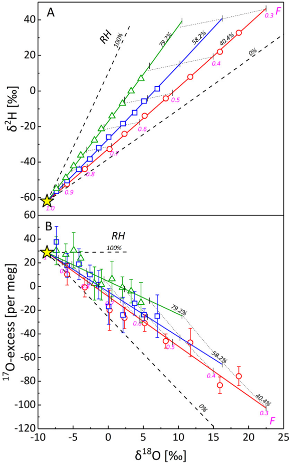
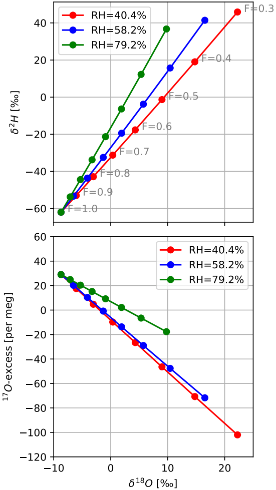


PySDM: model curves



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

[a] launch-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. ROZANSKI[1] 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)

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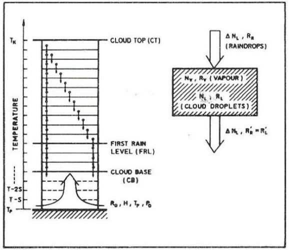

Fig. 3. Schematic diagram of the multibox cloud model. Input data: initial temperature, T_p; final temperature, T_k; initial pressure, P_0; relative humidity, H; initial isotopic composition of water vapour, R_0; cloud water mixing ratio, N_L; temperature step, S; isotope exchange factor, K.

Tellus 34 (1982), 2

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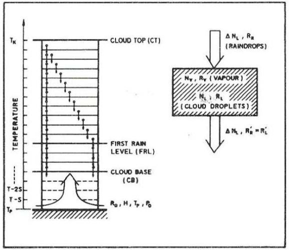

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Tellus 34 (1982), 2

- hydrostatic/adiabatic rainshaft with precip removal

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

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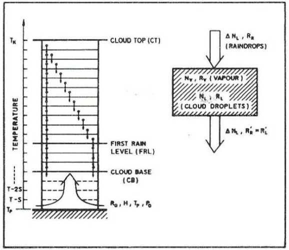

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Tellus 34 (1982), 2

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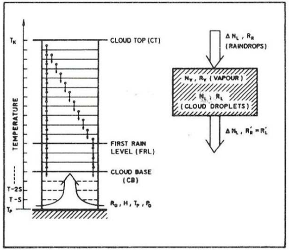

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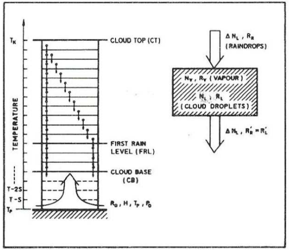

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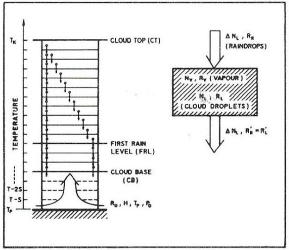

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- minimal model for capturing isotope exchange between precip, ambient vapor and cloud water ($\rightsquigarrow$ hypothesis explaining observed steep δ^2H profile gradients beyond condensation-only effects)

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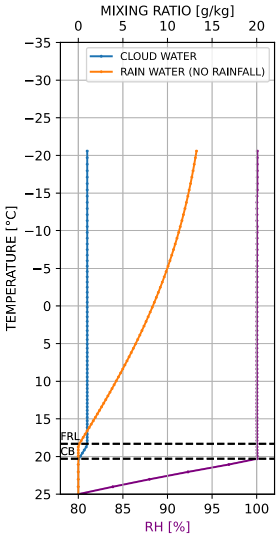

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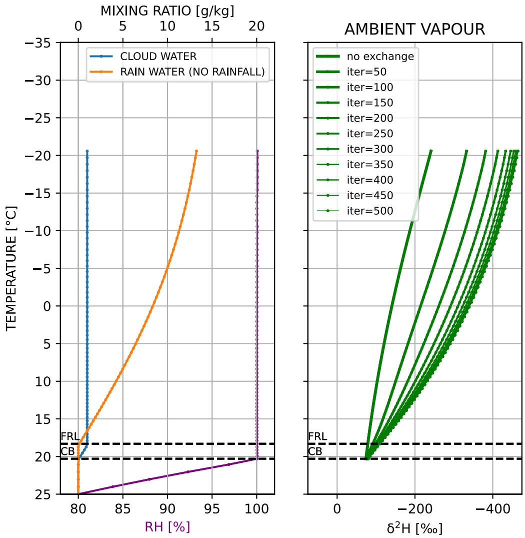

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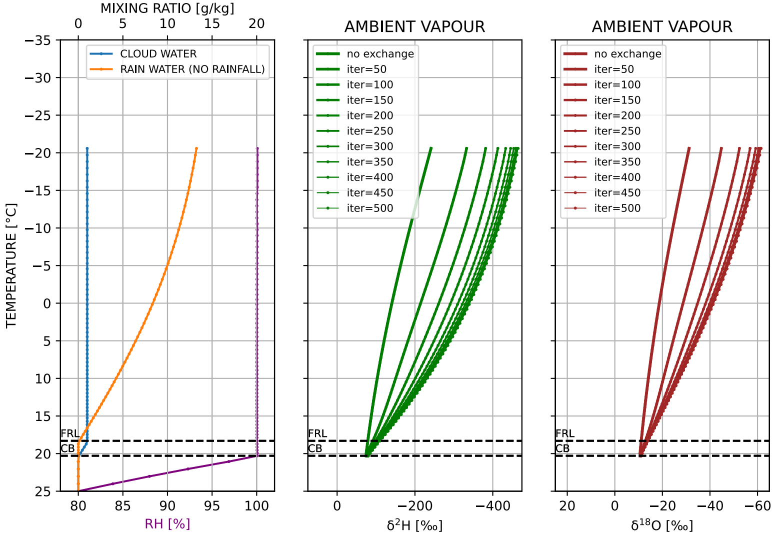

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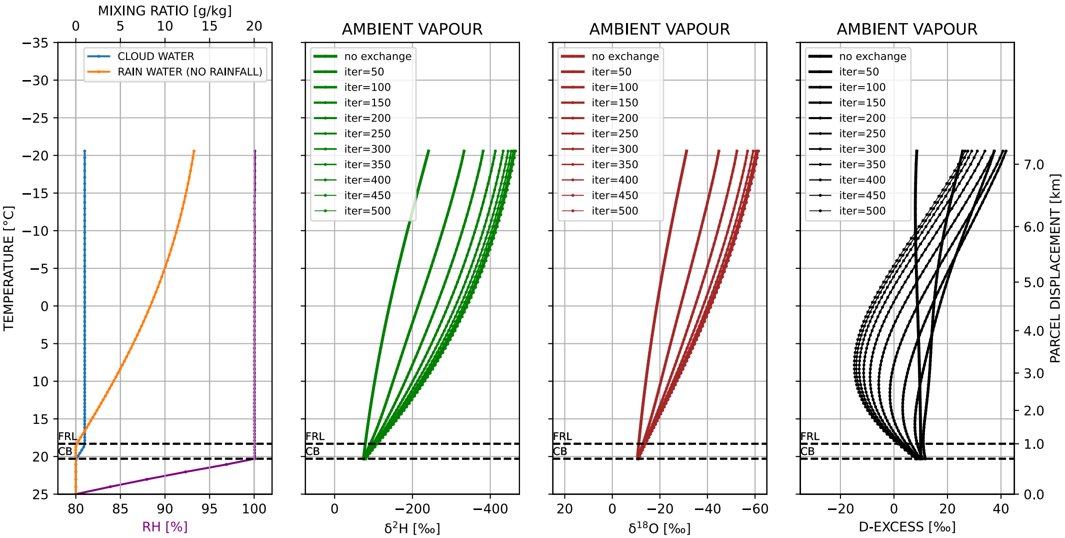

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- ice-phase processes

Thank you for your attention!

(sylwester.arabas@agh.edu.pl)

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