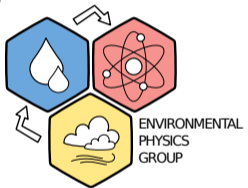


# A particle-based microphysics study of isotope exchanges in a single-column rain-shaft model

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



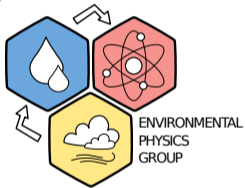
AGH University in Krakow, Poland





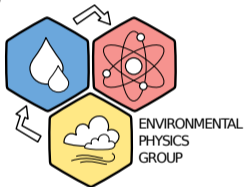
IAEA/GNIP site in Kraków





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

A screenshot of the IAEA website page for the Global Network of Isotopes in Precipitation (GNIP). The page features the IAEA logo and name at the top left, and navigation links for 'Press centre', 'Employment', and 'Contact' at the top right. Below the header is a search bar and a menu with options like 'TOPICS', 'SERVICES', 'RESOURCES', 'NEWS &amp; EVENTS', and 'ABOUT US'. The main content area has a blue header with the breadcrumb 'Home / Services / Networks / Global Network of Isotopes in Precipitation (GNIP)'. Below this is a large image of a water droplet falling into a pool of water. The title 'Global Network of Isotopes in Precipitation (GNIP)' is displayed in a white box over the image. A 'Networks' tab is active on the left. The main text describes GNIP as a worldwide isotope monitoring network of hydrogen and oxygen isotopes in precipitation, initiated in 1960 by the IAEA and WMO. A button labeled 'Access the Network' is located on the right side of the page.



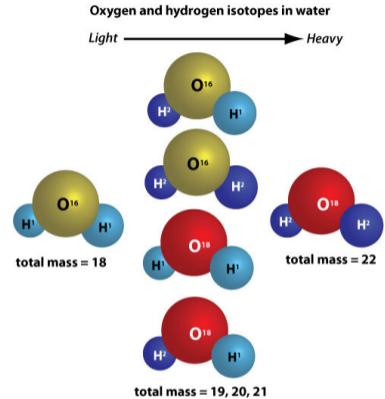
- ❑ IAEA/GNIP site in Kraków
- ❑ 50-year precip isotopic data record
- ❑ high-altitude lab (clouds in-situ)  
@Kasprowy Wierch (6500 ft AMSL)



photo: naukaoklimacie.pl

# clouds from a water isotopic point of view

- water isotopologues (stable):  $\text{H}_2\text{O}$  (99.7%),  $\text{H}_2^{18}\text{O}$  (0.2%),  $\text{H}_2^{17}\text{O}$  (0.04%),  $\text{HDO}$  (0.03%), ...

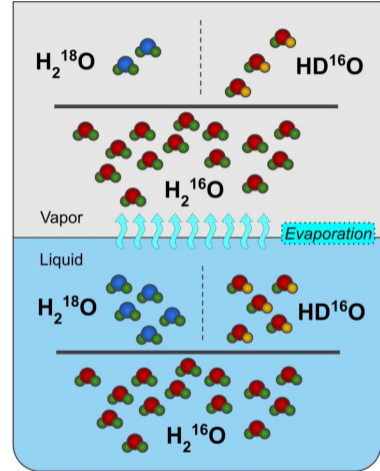


graphic: usgs.gov

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

# 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

# clouds from a water isotopic point of view

- ❏ water isotopologues (stable): H<sub>2</sub>O (99.7%), H<sub>2</sub><sup>18</sup>O (0.2%), H<sub>2</sub><sup>17</sup>O (0.04%), HDO (0.03%), ...
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- ❏ differences in diffusivity in air
  - ↪ non-equilibrium (kinetic) fractionation
  - ↪ applies to sub- and super-saturated conditions (+ liq/ice)
  - ↪ more pronounced for O than H

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

$\epsilon_{\text{kin}}$  kinetic fractionation coeff.

$n$  turbulence parameter

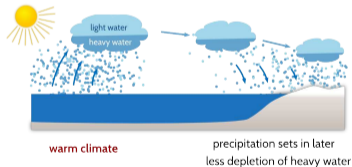
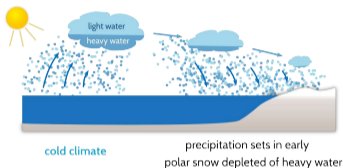
$\epsilon_{\text{diff}}$  diffusive fractionation coeff.

$RH$  rel. humidity



# clouds from a water isotopic point of view

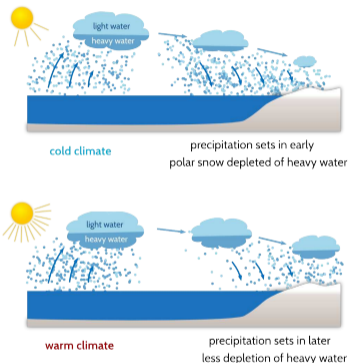
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  - ↪ more pronounced for O than H
- ❑ cloud  $\mu$ -physics shapes isotopic composition of “meteoric water”
  - ↪ data for validation of  $\mu$ -physical models!



graphic: physics-in-a-nutshell.com

# clouds from a water isotopic point of view

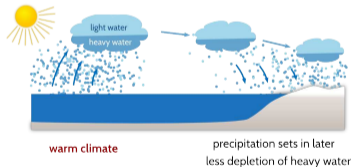
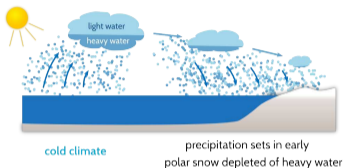
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- ❑ freezing “freezes” the isotopic composition of water



graphic: physics-in-a-nutshell.com

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- ❑ freezing “freezes” the isotopic composition of water
- ❑ isotope-aware  $\mu$ -physics models in ice isotopic data analysis



graphic: physics-in-a-nutshell.com

let's equip a particle-based  $\mu$ -physics package  
with isotope fractionation model!

# PySDM: open-source particle-based $\mu$ -physics modeling package



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## PySDM 2.40

✓ latest version

```
pip install PySDM
```

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 LLVM NumPy CUDA ThrustRTC Linux macOS Windows Jupyter

Maintained by OpenMined PySDM JOSS 10.21105/joss.03219 DOI 10.5281/zenodo.1204942

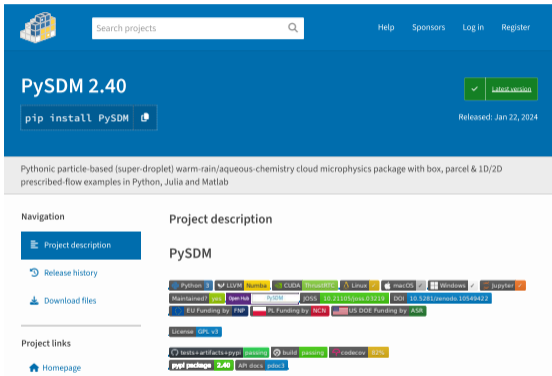
EU Funding by FPF NCH US DOE Funding by ASA

License [GPL v3](#)

tests+artifacts+pypp passing build passing collector 0.2%

pypi package **2.40** API docs pdoc3

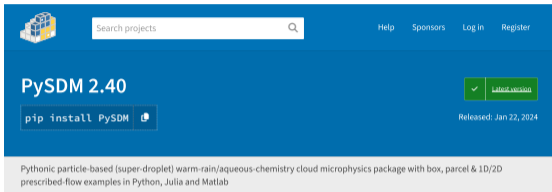
# PySDM: open-source particle-based $\mu$ -physics modeling package



The screenshot shows the GitHub repository page for PySDM. At the top, there is a search bar and navigation links for Help, Sponsors, Log in, and Register. The main header features the PySDM logo, the version number 'PySDM 2.40', and a 'latest version' button. Below this is a 'pip install PySDM' button and the release date 'Released: Jan 22, 2024'. A descriptive paragraph 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 contains navigation options: Project description (selected), Release history, and Download files. The main content area is titled 'Project description' and 'PySDM'. It includes a list of supported platforms (Python, LLVM, NumPy, CUDA, ThrustRTC, Linux, macOS, Windows, SuperMUC) and funding sources (EU, PL, US). At the bottom, there are badges for license (GPL v3), build status (passing), and coverage (82%).

particle diffusional growth/evaporation  
(incl. CCN activation)

# PySDM: open-source particle-based $\mu$ -physics modeling package



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## PySDM 2.40

✓ latest version

`pip install PySDM`

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

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

### Navigation

Project description

Release history

Download files

### Project links












Homepage

### Project description

#### PySDM

Python  LLVM  NumPy  CUDA  ThrustRTC  Linux  macOS  Windows  Jupyter 

Maintained by           

EU Funding by           

License 

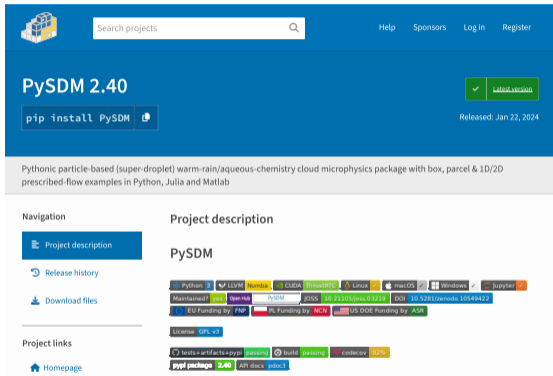
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- particle diffusional growth/evaporation (incl. CCN activation)
- collisional growth and breakup (Monte-Carlo, SDM)
- aqueous-phase oxidation of  $\text{SO}_2$  by  $\text{H}_2\text{O}_2$  and  $\text{O}_3$



# PySDM: open-source particle-based $\mu$ -physics modeling package



The screenshot shows the GitHub repository page for PySDM. At the top, there is a search bar and navigation links for Help, Sponsors, Log in, and Register. The main header features the PySDM 2.40 logo, a 'latest version' badge, and a 'pip install PySDM' button. Below this, a brief 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 page is divided into 'Navigation' (Project description, Release history, Download files) and 'Project links' (Homepage). The 'Project description' section includes a 'Project description' heading, the name 'PySDM', and a row of platform compatibility badges (Python, LLVM, NumPy, CUDA, ThrustRTC, Linux, macOS, Windows, SuperMIPAS). Below these are badges for 'Maintained', 'Open Hub', 'PyPI', 'DOI', and 'Downloads'. Funding sources for the EU, PL, and US are also listed. At the bottom, there are badges for 'License: GPL v3', 'Tests + artifacts + pypp', 'Build', 'Passing', 'Collective', and 'PyPI package 2.40'.

- particle diffusional growth/evaporation (incl. CCN activation)
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- aqueous-phase oxidation of  $\text{SO}_2$  by  $\text{H}_2\text{O}_2$  and  $\text{O}_3$
- immersion freezing (Monte-Carlo, ABIFM)

# PySDM: open-source particle-based $\mu$ -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 links

- Homepage

### Project description

#### PySDM

Python LLVM NumPy CUDA ThrustRTC Linux macOS Windows SuperMIPED

watched open issues pull requests downloads

EU Funding by FWF PL Funding by NCH US DOE Funding by ASA

License GPL v3

tests+artifacts+pypp passing build passing collect 0.2%

pypi package 2.40 API docs v2.40

- particle diffusional growth/evaporation (incl. CCN activation)
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- immersion freezing (Monte-Carlo, ABIFM)
- features 0D, 1D and 2D example simulation setups

# PySDM: open-source particle-based $\mu$ -physics modeling package

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## PySDM 2.40

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

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### Project description

#### PySDM

Python LLVM Numba CUDA ThrustRTC Linux macOS Windows SuperMUC

maintained by OpenMeteo PySDM 3955 10 21105 (size 0.3219) DOI 10.5281/zenodo.12049422

EU Funding by FWF PL Funding by NCB US DOE Funding by ASA

License GPL v3

tests-artifacts+pypp passing build passing coverage 82%

pypp package 2.40 API docs pdox3

- particle diffusional growth/evaporation (incl. CCN activation)
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- 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
<b>formulae-only</b>								
Pierchala et al. 2022			x					#lab-experiment
<b>OD box environment</b>								
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
<b>OD parcel environment</b>								
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							#timescales
Jaruga & Pawlowska 2018	x					x		#Hoppel-gap
Yang et al. 2018	x							#ripening
Lowe et al. 2019	x							#surfactants
Grabowski and Pawlowska 2023	x							#ripening
<b>1D single-column kinematic env.</b>								
Shipway & Hill 2012	x	x			x			#KiD
deJong et al. 2023 (figures 6-8)	x	x		x	x			#KiD
<b>2D prescribed-flow environment</b>								
Arabas et al. 2015	x	x			x			#GUI
Arabas et al. 2023 (figure 11)	x	x			x		x	#Paraview

<sup>a</sup>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](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](https://doi.org/10.1016/j.gca.2022.01.020)

Geochimica et Cosmochimica Acta 322 (2022) 244–259

[www.elsevier.com/locate/gca](http://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

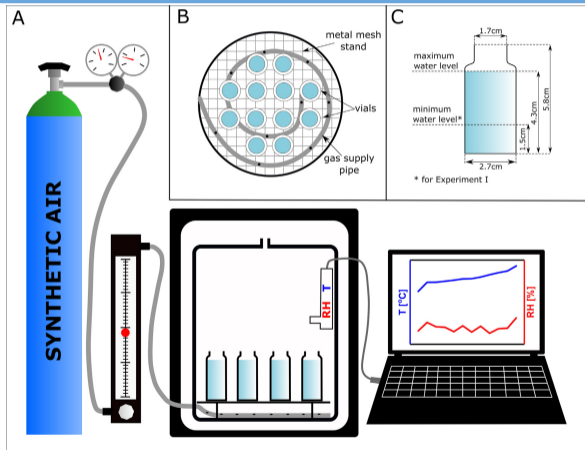
Anna Pierchala<sup>\*</sup>, Kazimierz Rozanski, Marek Dulinski, Zbigniew Gorczyca

*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

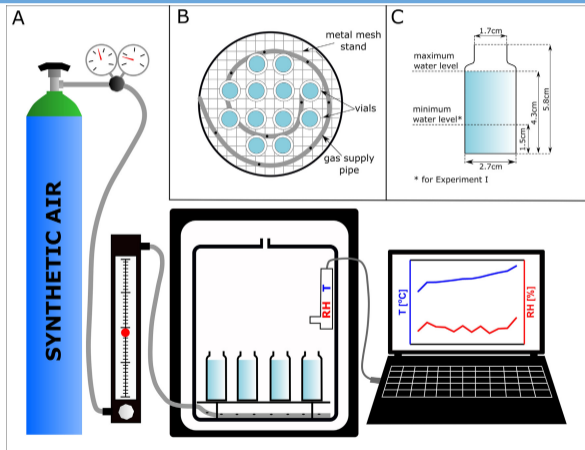
<sup>a</sup>launch-in-the-cloud URL: [https://mybinder.org/v2/gh/open-atmos/PySDM.git/main?urlpath=lab/tree/examples/PySDM\\_examples/Pierchala\\_et\\_al\\_2022](https://mybinder.org/v2/gh/open-atmos/PySDM.git/main?urlpath=lab/tree/examples/PySDM_examples/Pierchala_et_al_2022)

Fig. 1 (paper): lab experiment setup



<sup>a</sup>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](https://mybinder.org/v2/gh/open-atmos/PySDM.git/main?urlpath=lab/tree/examples/PySDM_examples/Pierchala_et_al_2022)

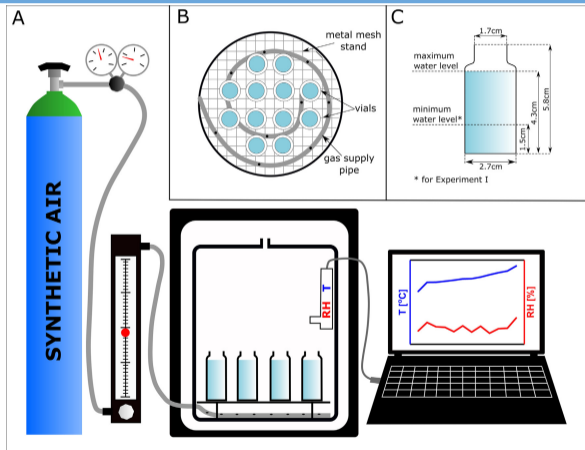
Fig. 1 (paper): lab experiment setup



fractionation upon evaporation  
(incl. kinetic effects)

<sup>a</sup>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](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



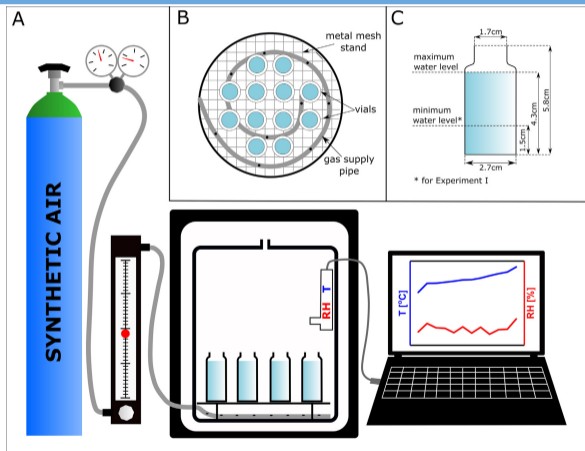
❑ fractionation upon evaporation  
(incl. kinetic effects)

❑ multi-day experiments  
(up to two weeks)



<sup>a</sup>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](https://mybinder.org/v2/gh/open-atmos/PySDM.git/main?urlpath=lab/tree/examples/PySDM_examples/Pierchala_et_al_2022)

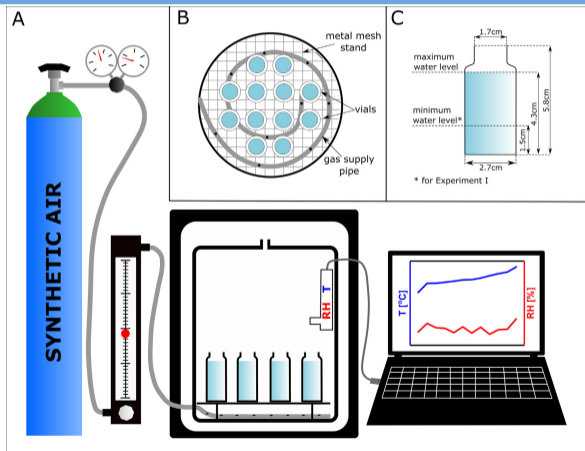
Fig. 1 (paper): lab experiment setup



- fractionation upon evaporation (incl. kinetic effects)
- multi-day experiments (up to two weeks)
- Picarro L2140-i cavity ring-down laser spectrometer (D,  $^{18}\text{O}$ ,  $^{17}\text{O}$ ) (probing vaporized water)

<sup>a</sup>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](https://mybinder.org/v2/gh/open-atmos/PySDM.git/main?urlpath=lab/tree/examples/PySDM_examples/Pierchala_et_al_2022)

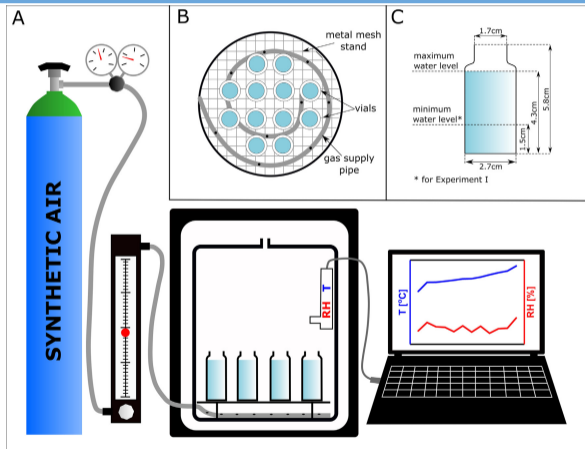
Fig. 1 (paper): lab experiment setup



- ❑ fractionation upon evaporation (incl. kinetic effects)
- ❑ multi-day experiments (up to two weeks)
- ❑ Picarro L2140-i cavity ring-down laser spectrometer (D,  $^{18}\text{O}$ ,  $^{17}\text{O}$ ) (probing vaporized water)
- ❑ constant T/RH, variable T or variable RH setups

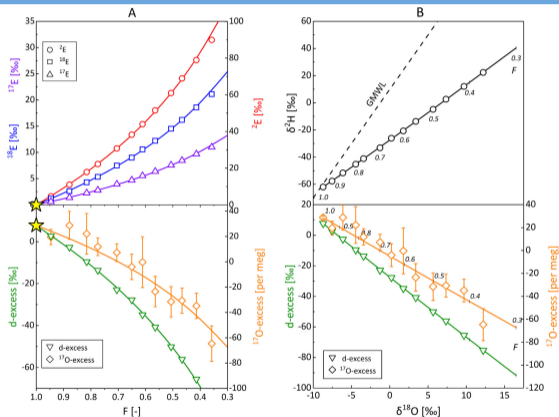
<sup>a</sup>launch-in-the-cloud URL: [https://mybinder.org/v2/gh/open-atmos/PySDM.git/main?urlpath=lab/tree/examples/PySDM\\_examples/Pierchala\\_et\\_al\\_2022](https://mybinder.org/v2/gh/open-atmos/PySDM.git/main?urlpath=lab/tree/examples/PySDM_examples/Pierchala_et_al_2022)

Fig. 1 (paper): lab experiment setup



- ❑ fractionation upon evaporation (incl. kinetic effects)
- ❑ multi-day experiments (up to two weeks)
- ❑ Picarro L2140-i cavity ring-down laser spectrometer (D,  $^{18}\text{O}$ ,  $^{17}\text{O}$ ) (probing vaporized water)
- ❑ constant T/RH, variable T or variable RH setups
- ❑ analysis against Rayleigh distillation + Craig-Gordon RH-dependence

Fig. 3 (paper): measurements + model



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

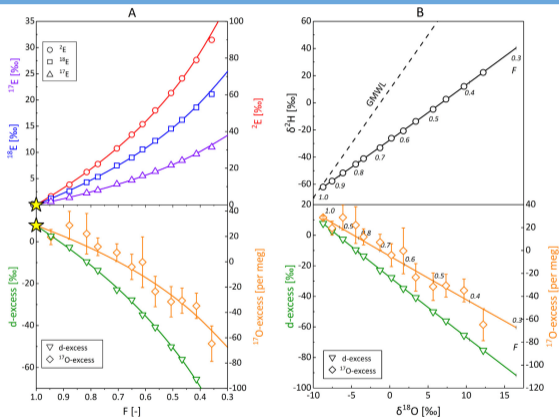
$$\delta = \frac{[\text{heavy iso.}]}{[\text{light iso.}]} \Big|_{\text{VSMOW}} - 1$$

F: fraction of water remaining

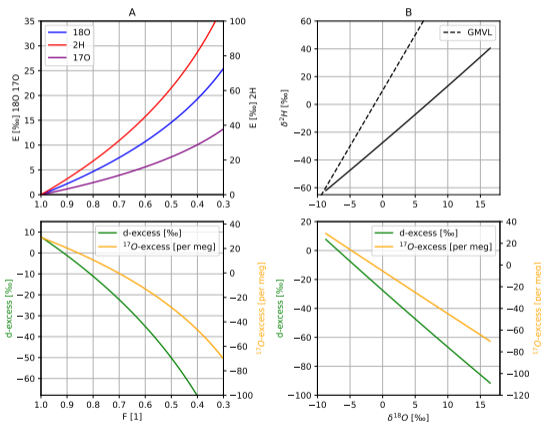
$$d\text{-excess: } \delta^2\text{H} - 8 \cdot \delta^{18}\text{O}$$

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

Fig. 3 (paper): measurements + model



PySDM: theoretical curves



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

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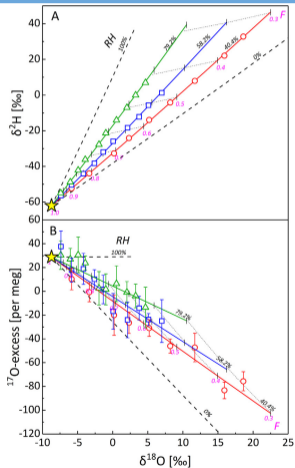
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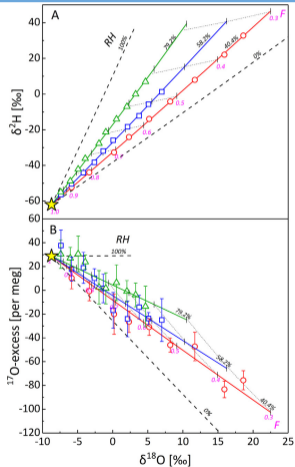
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Fig. 4 (paper): RH varied

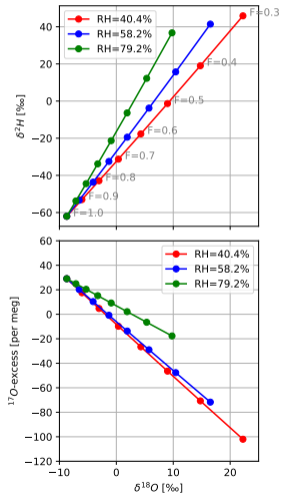


<sup>a</sup>launch-in-the-cloud URL: [https://mybinder.org/v2/gh/open-atmos/PySDM.git/main?urlpath=lab/tree/examples/PySDM\\_examples/Pierchala\\_et\\_al\\_2022](https://mybinder.org/v2/gh/open-atmos/PySDM.git/main?urlpath=lab/tree/examples/PySDM_examples/Pierchala_et_al_2022)

Fig. 4 (paper): RH varied



PySDM: model curves



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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<sup>1</sup> 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<sup>a</sup>

<sup>a</sup>launch-in-the-cloud URL: [https://mybinder.org/v2/gh/slayoo/PySDM.git/isotopes\\_rozanski\\_and\\_sonntag\\_example?urlpath=lab/tree/examples/PySDM\\_examples](https://mybinder.org/v2/gh/slayoo/PySDM.git/isotopes_rozanski_and_sonntag_example?urlpath=lab/tree/examples/PySDM_examples)

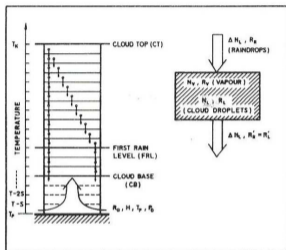
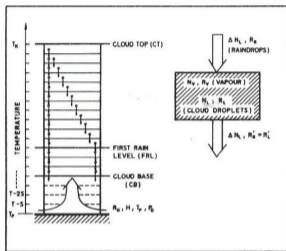


Fig. 3. Schematic diagram of the multibox cloud model. Input data: initial temperature,  $T_p$ ; final temperature,  $T_k$ ; initial pressure,  $P_0$ ; relative humidity,  $H$ ; initial isotopic composition of water vapour,  $R_0$ ; cloud water mixing ratio,  $N_L$ ; temperature step,  $S$ ; isotope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

Tellus 34 (1982), 2

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❖ hydrostatic/adiabatic rainshaft with precip removal

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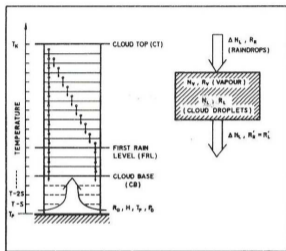


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Tellus 34 (1982), 2

- hydrostatic/adiabatic rainshaft with precip removal
- condensation: saturation adjustment

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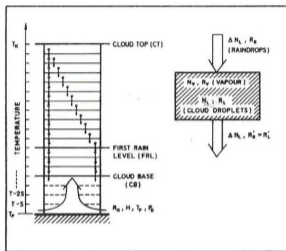


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Tellus 34 (1982), 2

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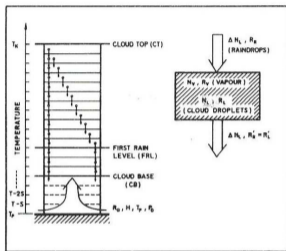


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Tellus 34 (1982), 2

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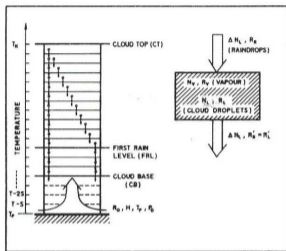


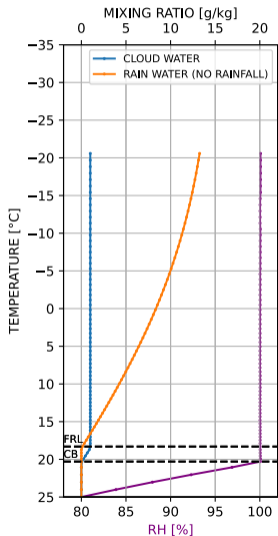
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Tellus 34 (1982), 2

- ❖ hydrostatic/adiabatic rainshaft with precip removal
- ❖ condensation: saturation adjustment
- ❖ rain formation: liquid water content threshold
- ❖ parcel-model iterations towards stationary state (no explicit role of time)
- ❖ 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)

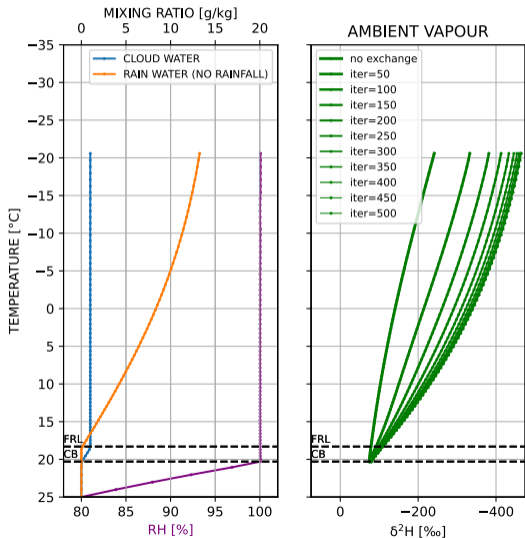
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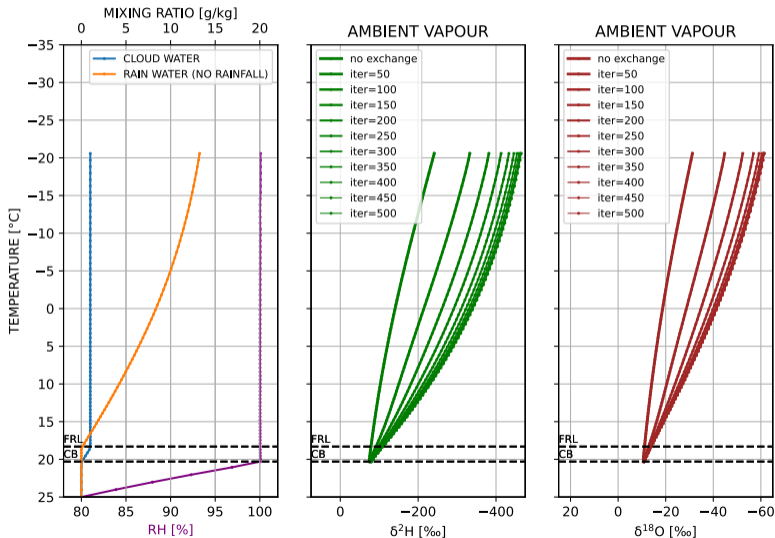
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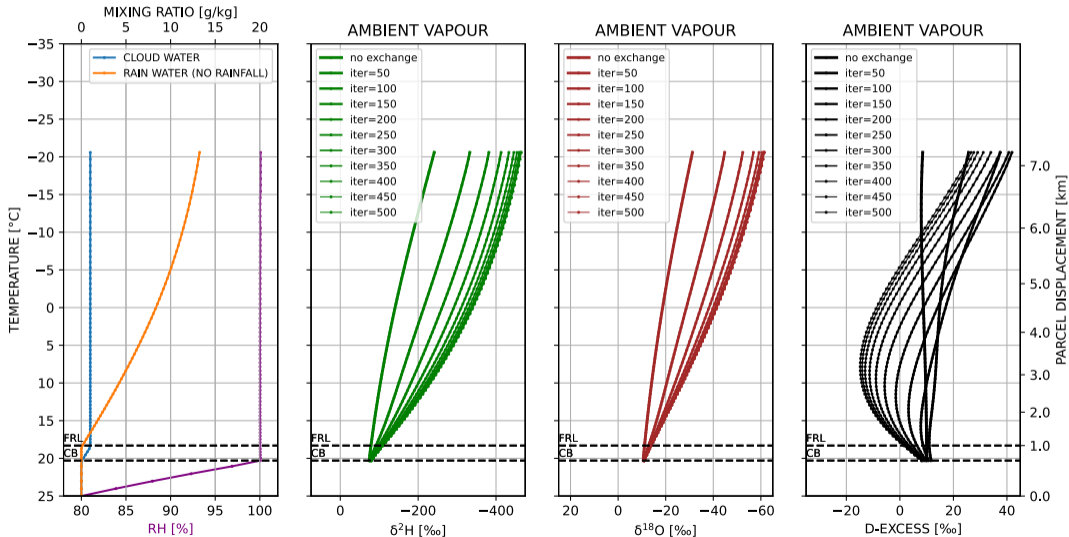
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# water isotopes in PySDM: summary, next steps

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

- ❑ **base SD attributes:** #moles of heavy isotopologue

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- ❑ ventilation and drop heat budget
- ❑ exploring dependence on droplet and precip size spectra (and hence aerosol)
- ❑ ice-phase processes

# Thank you for your attention!

(sylwester.arabas@agh.edu.pl)



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