

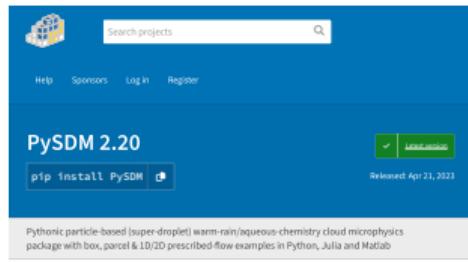
Modelling of water isotopic fractionation within and below clouds

Sylwester Arabas



AGH University in Krakow

github.com/open-atmos



PySDM 2.20

Released Apr 21, 2023

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

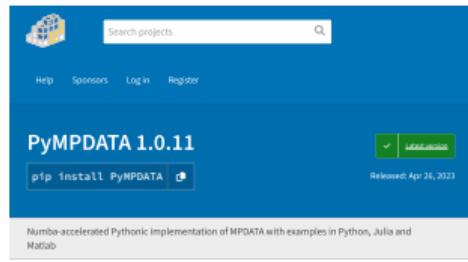
- Project description
- Release history
- Download files

Project links

- Homepage
- Documentation
- Source
- Tracker

Statistics

- Github statistics:
- Stars: 40
- Forks: 23
- Open issues: 101
- Open PRs: 13



PyMPDATA 1.0.11

Released Apr 26, 2023

pip install PyMPDATA

Numba-accelerated Pythonic implementation of MPDATA with examples in Python, Julia and Matlab

Navigation

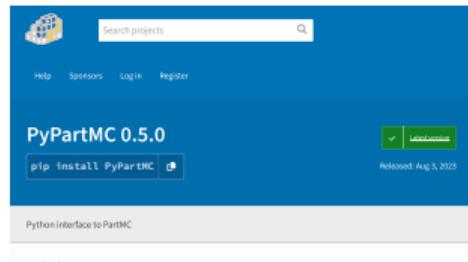
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Statistics

- Github statistics:
- Stars: 19
- Forks: 10
- Open issues: 25
- Open PRs: 3



PyPartMC 0.5.0

Released Aug 3, 2023

pip install PyPartMC

Python interface to PartMC

Navigation

- Project description
- Release history
- Download files

Project links

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- Source
- Tracker

Statistics

- Github statistics:
- Stars: 15
- Forks: 6
- Open issues: 54
- Open PRs: 3

Research Article

The super-droplet method for the numerical simulation of clouds and precipitation: a particle-based and probabilistic microphysics model coupled with a non-hydrostatic model

S. Shima ✉, K. Kusano, A. Kawano, T. Sugiyama, S. Kawahara

First published: 19 June 2009 | <https://doi.org/10.1002/qj.441> | Citations: 150

Abstract

A novel, particle-based, probabilistic approach for the simulation of cloud microphysics is proposed, which is named the super-droplet method (SDM). This method enables the accurate simulation of cloud microphysics with a less demanding cost in computation. SDM is applied to a warm-cloud system, which incorporates sedimentation, condensation/evaporation and stochastic coalescence. The methodology to couple super-droplets and a non-hydrostatic model is also developed. It is confirmed that the result of our Monte Carlo scheme for the stochastic coalescence of super-droplets agrees fairly well with the solutions of the stochastic coalescence equation. The behaviour of the model is evaluated using a simple test problem, that of a shallow maritime cumulus formation initiated by a warm bubble. Possible extensions of SDM are briefly discussed. A theoretical analysis suggests that the computational cost of SDM becomes lower than the spectral (bin) method when the number of attributes—the variables that identify the state of each super-droplet—becomes larger than some critical value, which we estimate to be in the range $2 \sim 4$.

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PySDM: open-source particle-based cloud-microphysics package

The screenshot shows the GitHub repository page for PySDM. It includes sections for Python 3, LLVM, Numba, CUDA, ThrustRTC, Linux, macOS, Windows, Jupyter, maintenance status (yes), Open Hub, EU Funding by FNP, PL Funding by NCN, US DOE Funding by ASR, License (GPL v3), test status (tests+artifacts+pypi: passing, build: passing, codecov: 84%), pypi package (2.54), API docs (pdoc3), and GitHub statistics (stars: 51, watching: 5, forks: 28).

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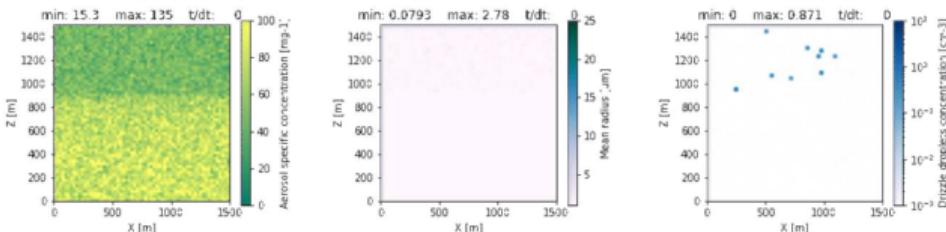
- [Bartman et al. 2022](#) (PySDM v1).
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51 stars

5 watching

28 forks

Report repository

Releases 86

PySDM v2.56 Latest
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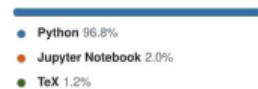
+ 85 releases

Contributors 19



+ 5 contributors

Languages



PySDM: open-source particle-based cloud-microphysics package

Python 3 LLVM Numba CUDA ThrustRTC Linux macOS Windows Jupyter Maintained? yes Open Hub PySDM
JOSS 10.21105/joss.03219 DOI 10.5281/zenodo.11186158
EU Funding by FNP PL Funding by NCN US DOE Funding by ASR
License GPL v3
tests+artifacts+pypi passing build passing codecov 84%
pypi package 2.54 API docs pdoc3

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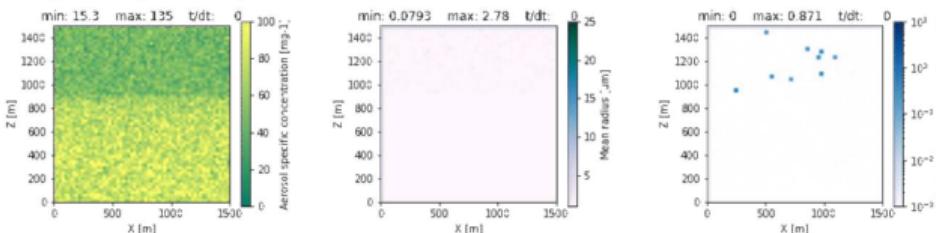
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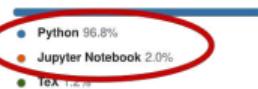
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Python 3 LLVM Numba CUDA ThrustRTC Linux macOS Windows Jupyter Maintained? yes Open Hub PySDM
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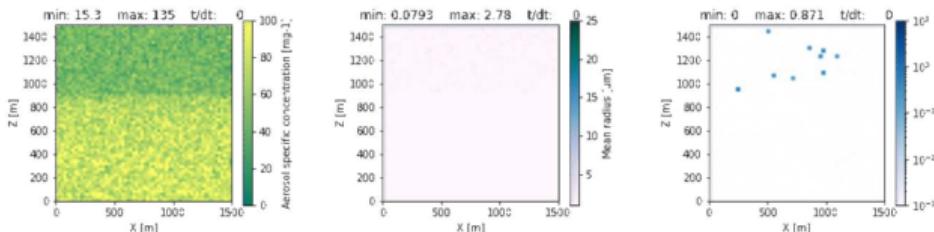
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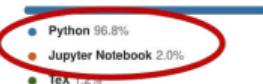
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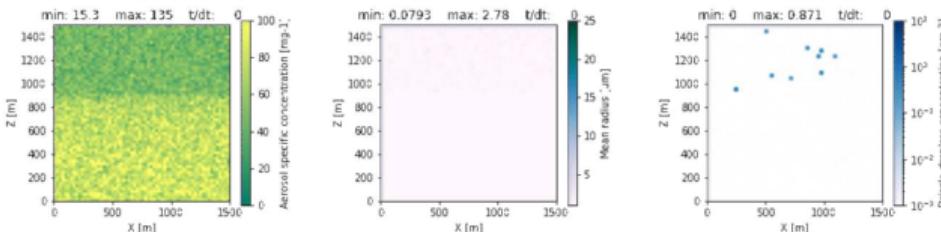
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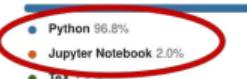
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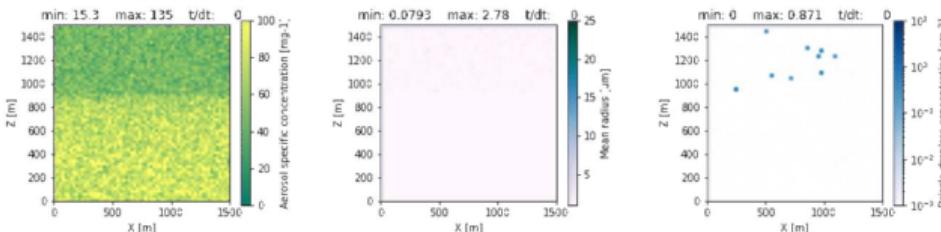
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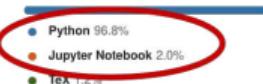
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Languages



PySDM: open-source particle-based cloud-microphysics package

The screenshot shows the GitHub profile of the PySDM repository. It includes sections for programming languages (Python 3, LLVM, CUDA, ThrustRTC, Linux, macOS, Windows), maintained status (Jupyter, Maintained? yes), funding (EU, PL, US DOE), license (GPL v3), and build status (tests+artifacts+pypi passing, build pass, codecov 84%).

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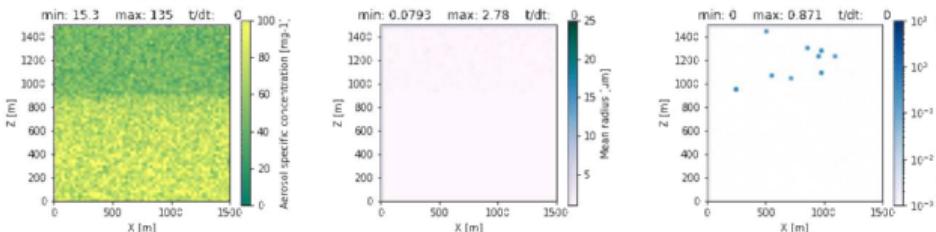
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Languages

Python 96.8%
Jupyter Notebook 2.0%
TeX 1.2%

PySDM: open-source particle-based cloud-microphysics package

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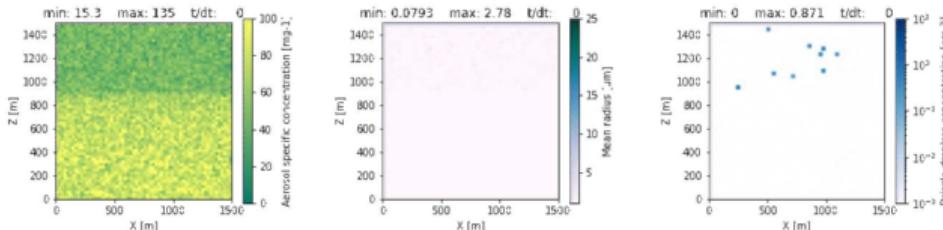
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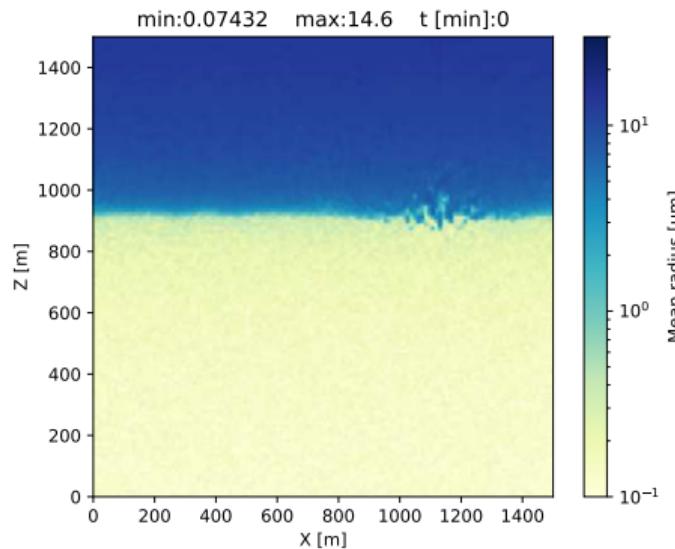
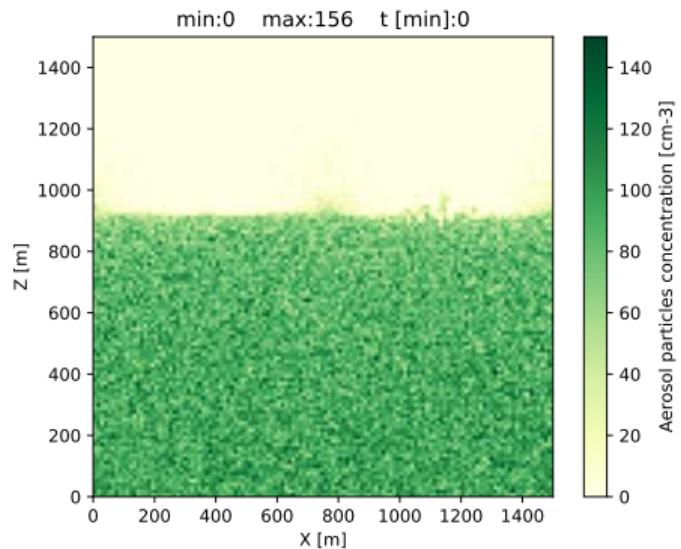


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Languages

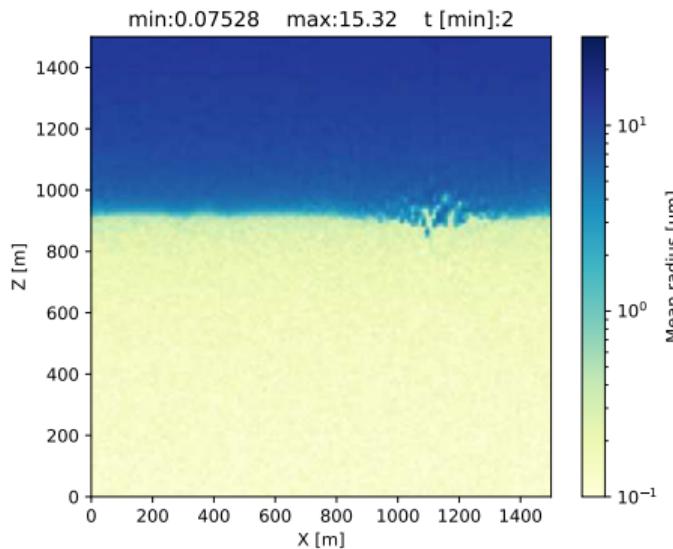
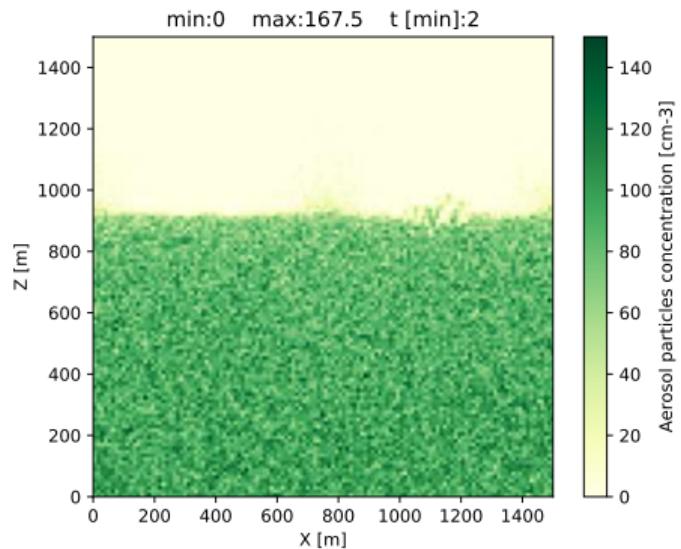
Python 96.8%
Jupyter Notebook 2.0%
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Eulerian solver (kinematic flow) grid: 128×128
Lagrangian super-particles population: 2^{21}



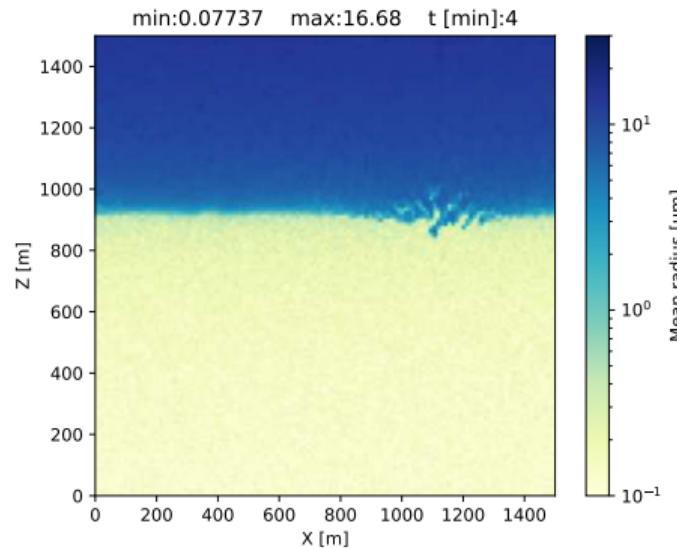
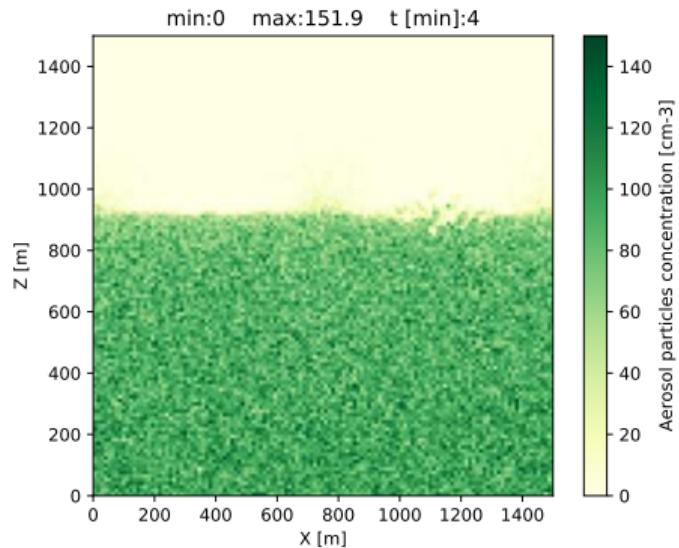
simulation & vis.: Piotr Bartman

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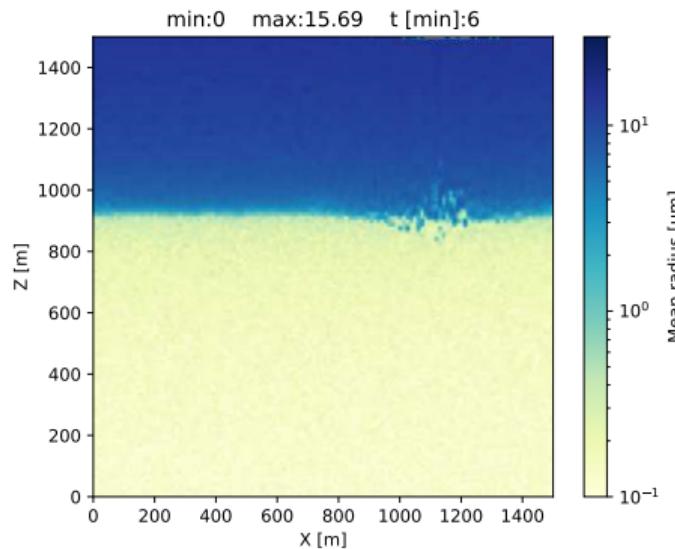
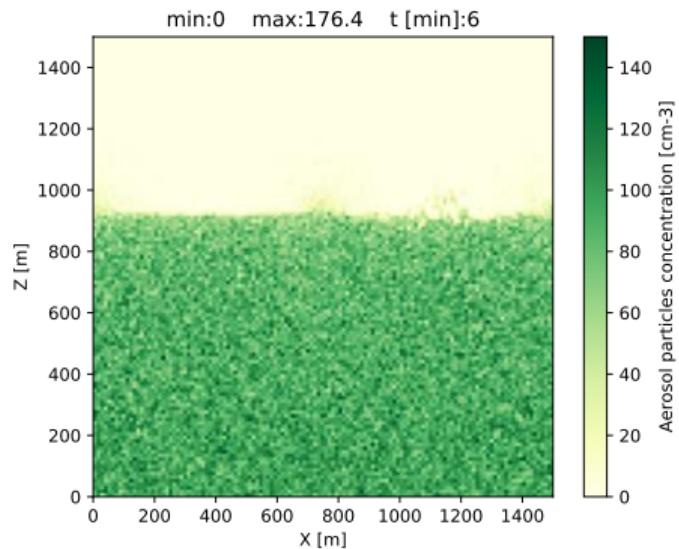
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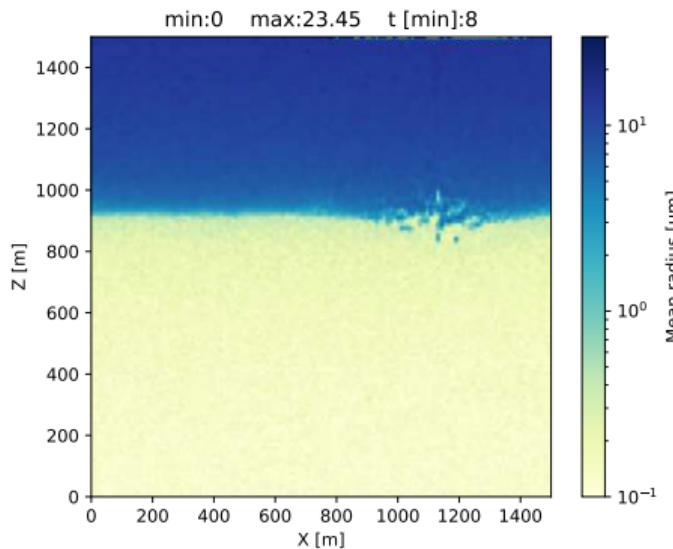
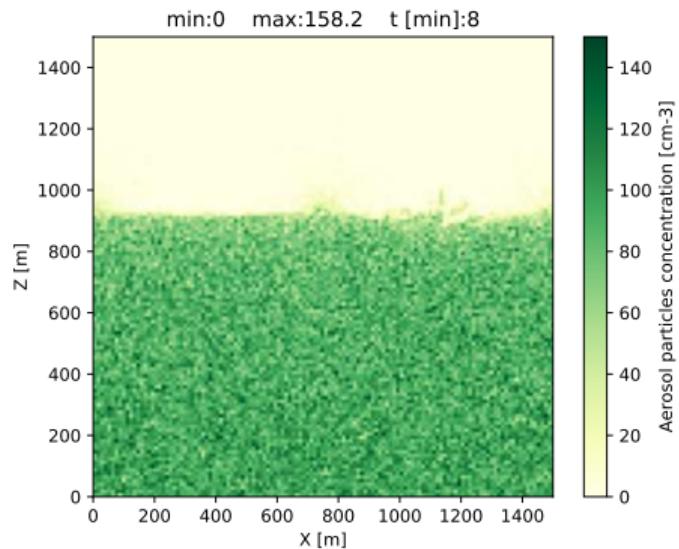
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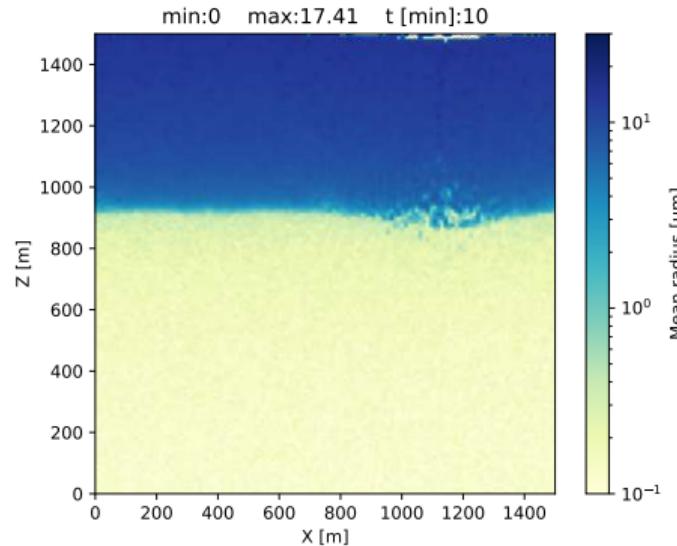
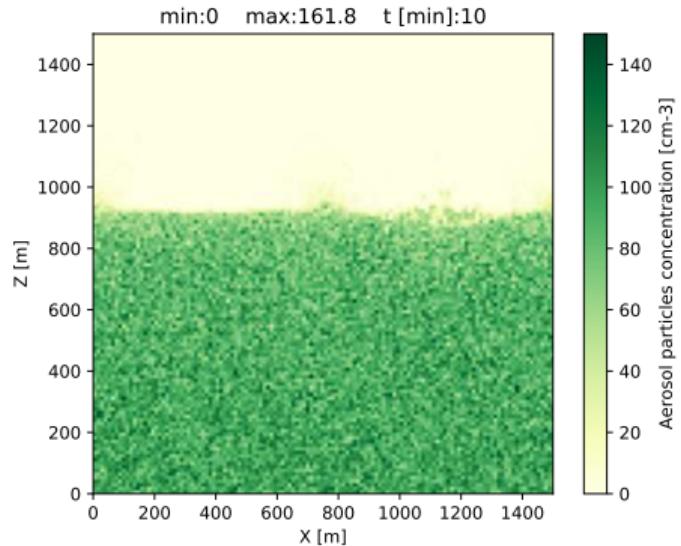
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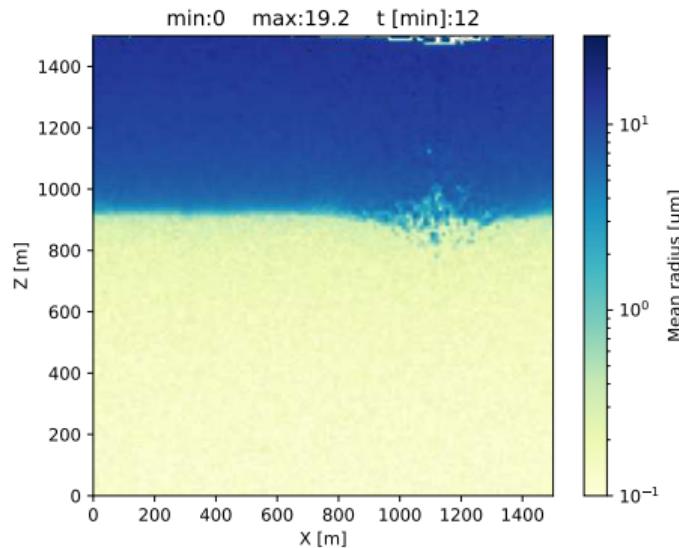
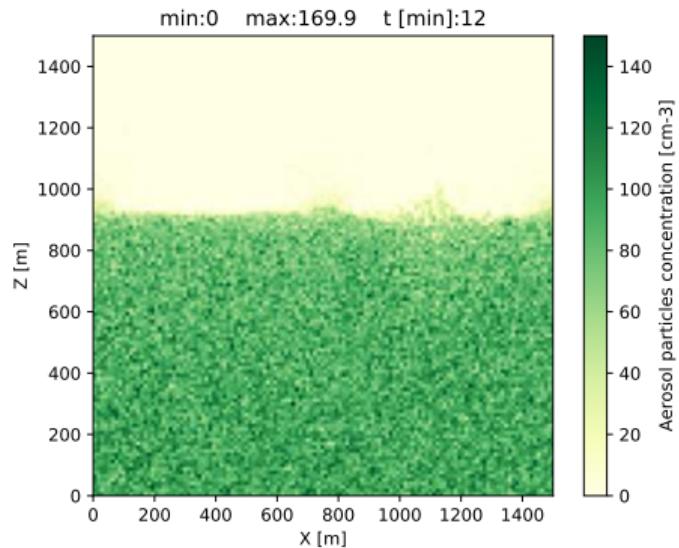
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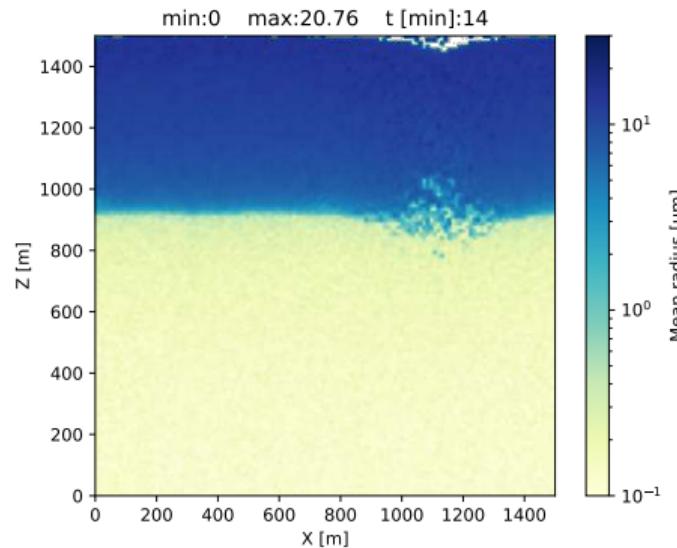
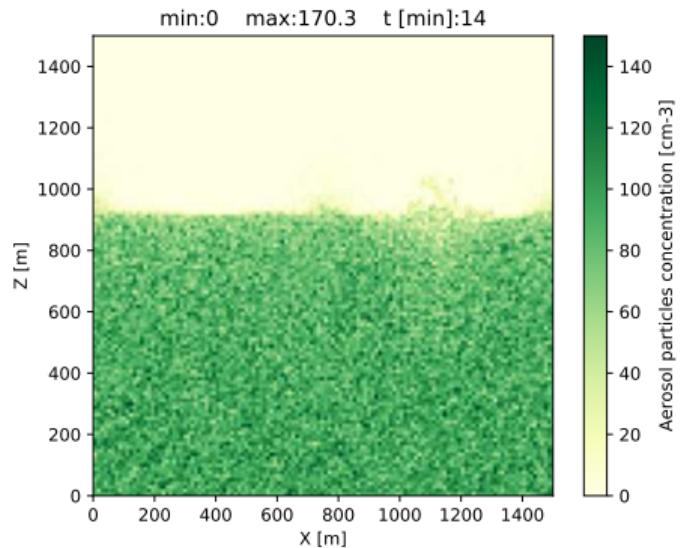
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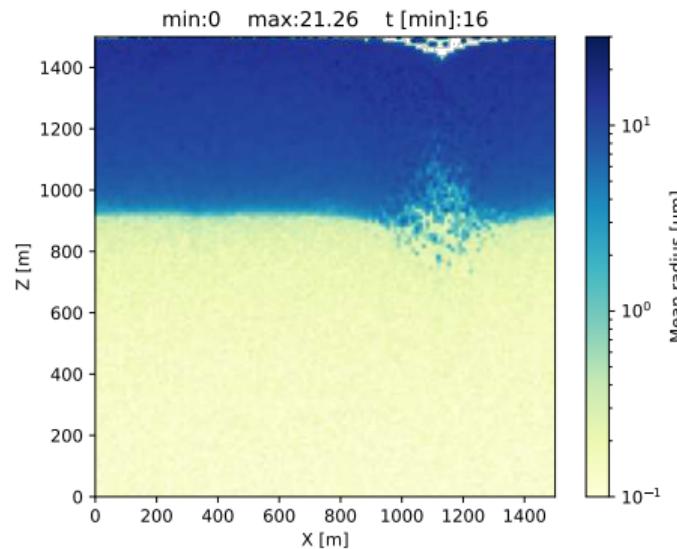
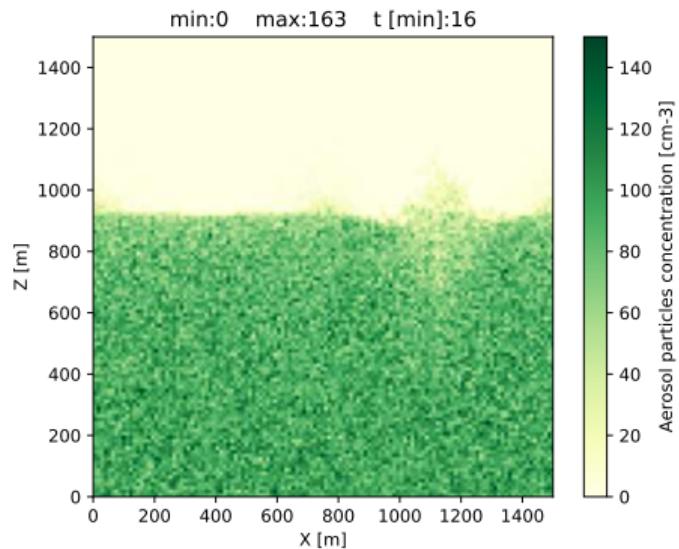
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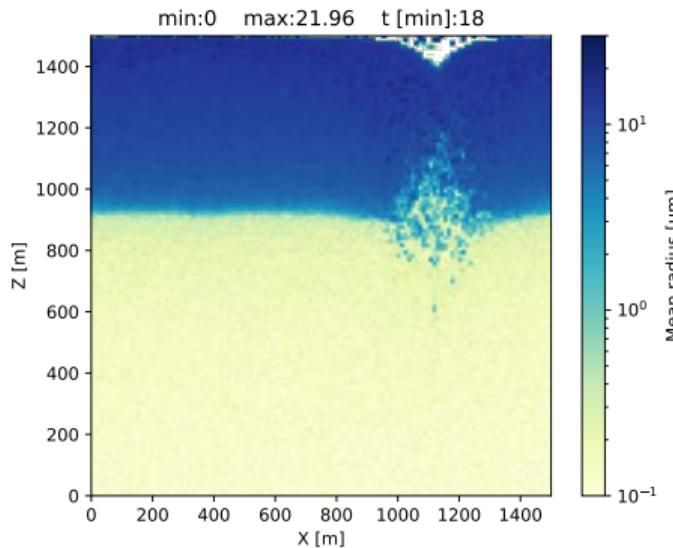
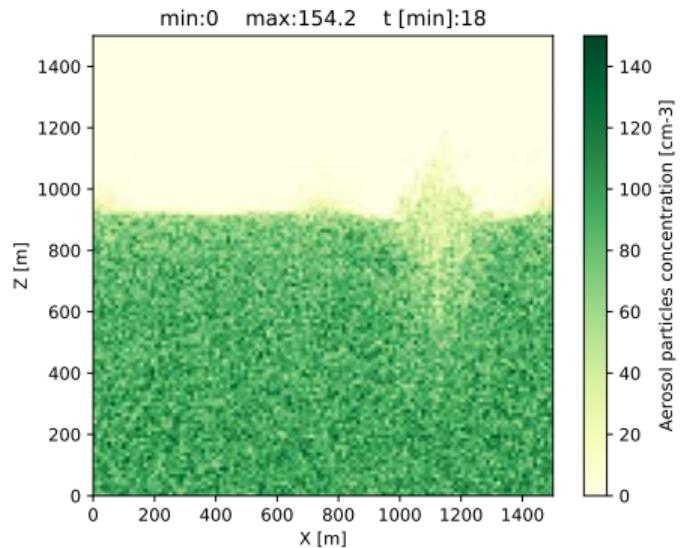
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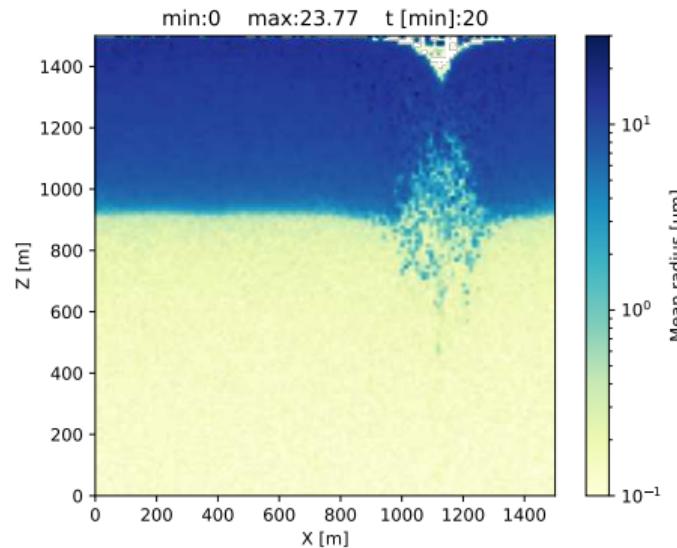
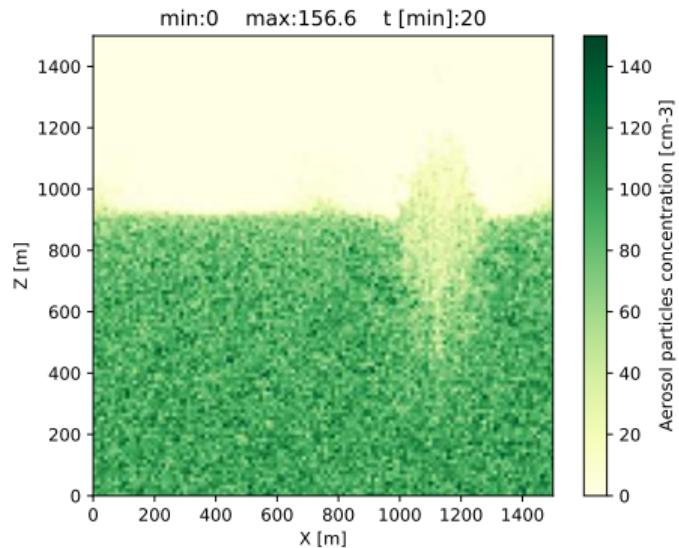
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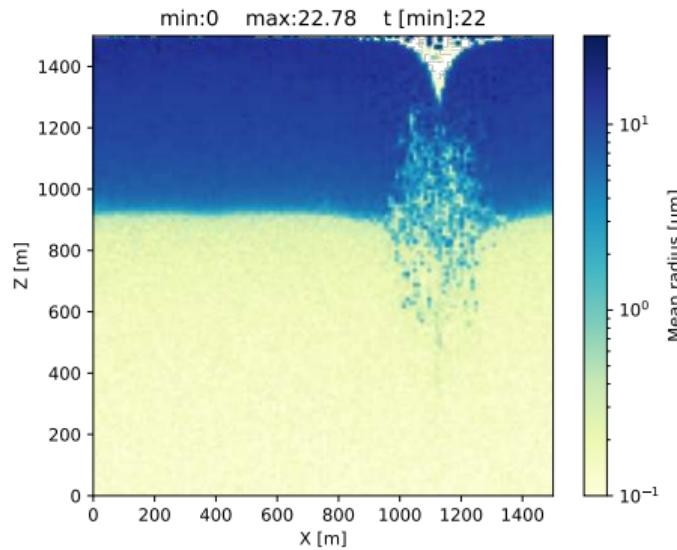
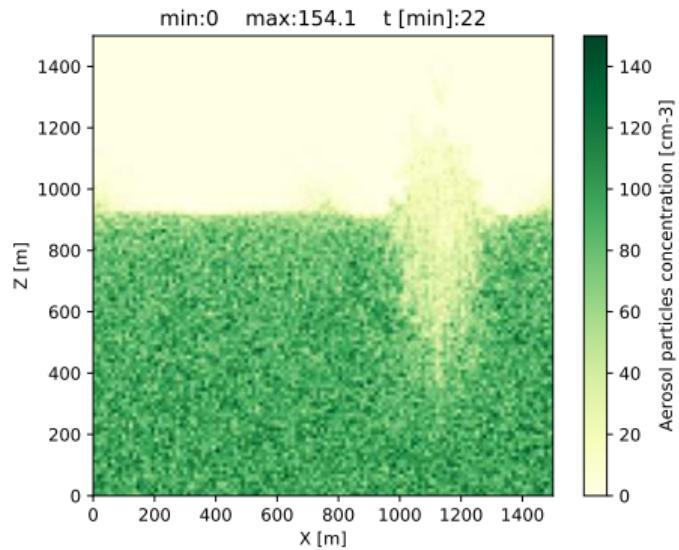
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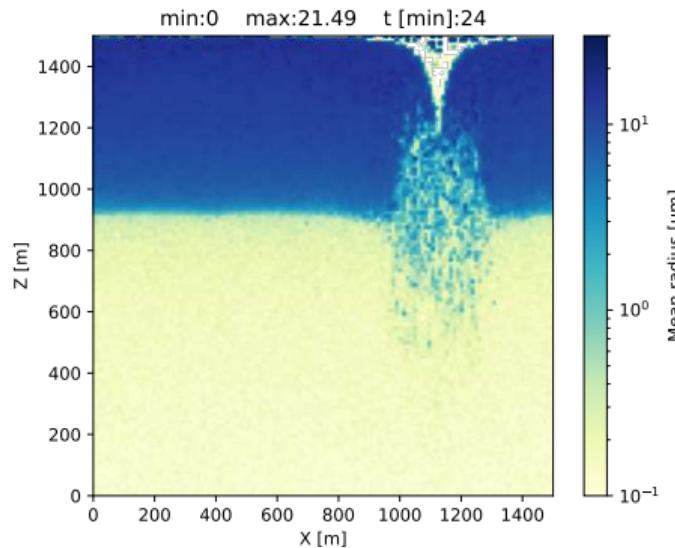
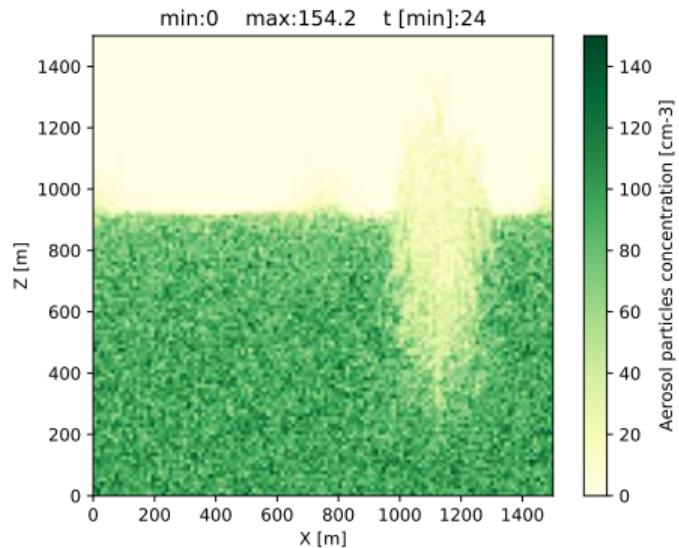
simulation & vis.: Piotr Bartman

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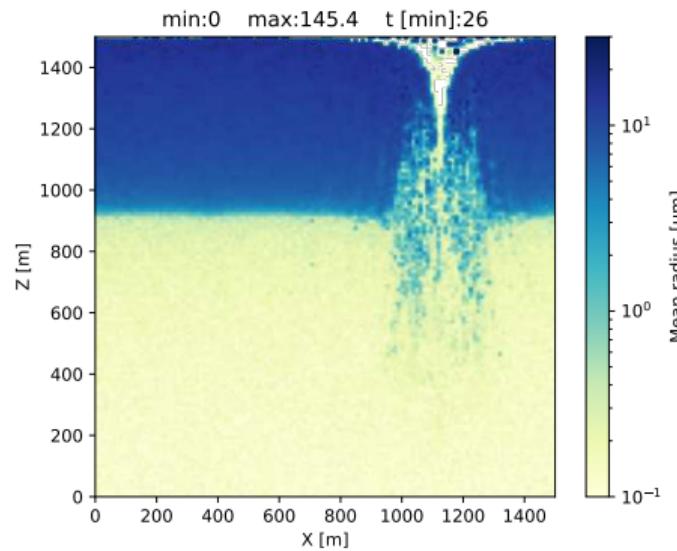
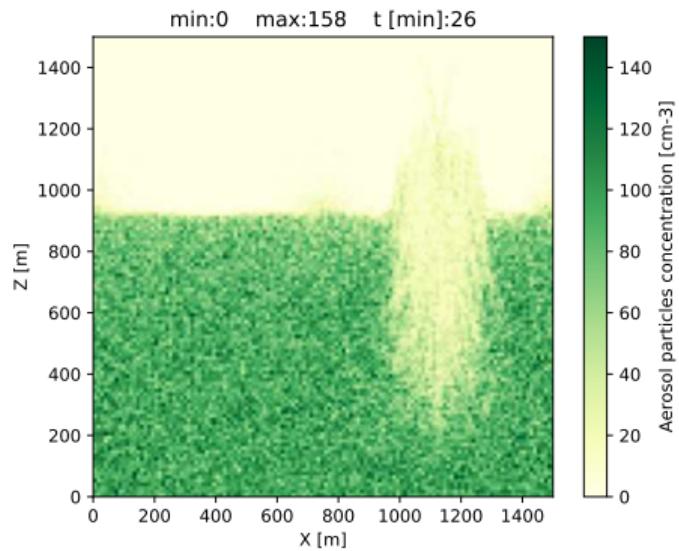
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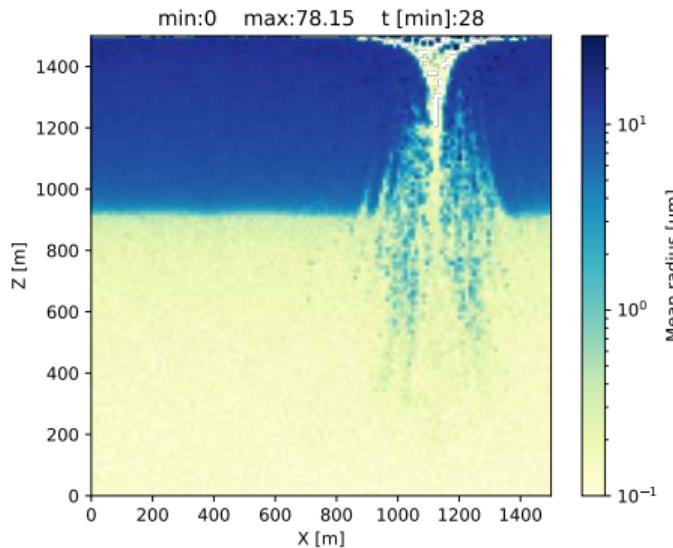
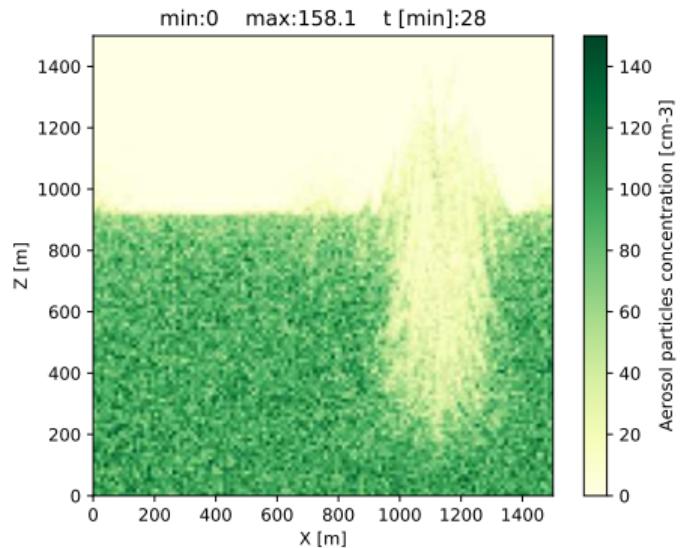
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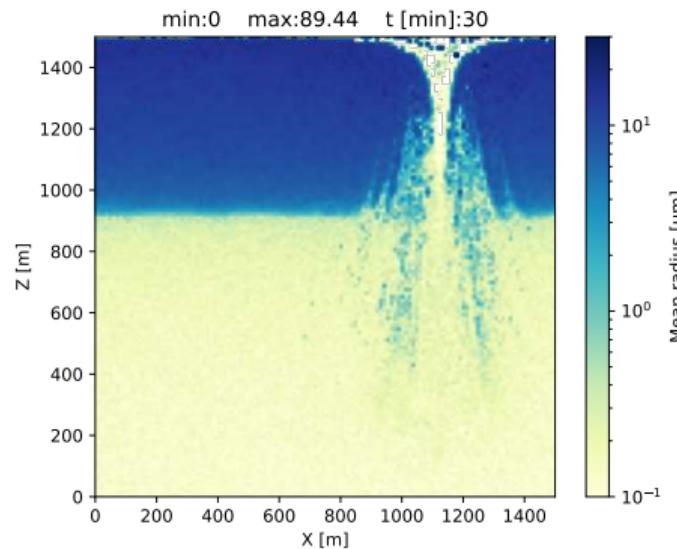
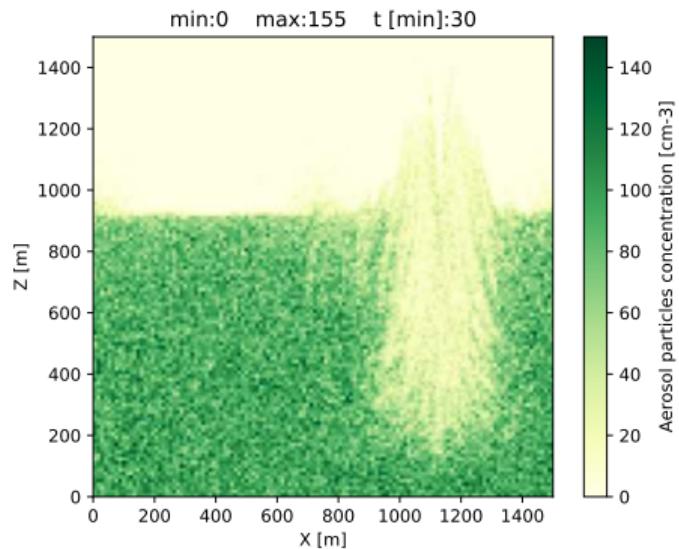
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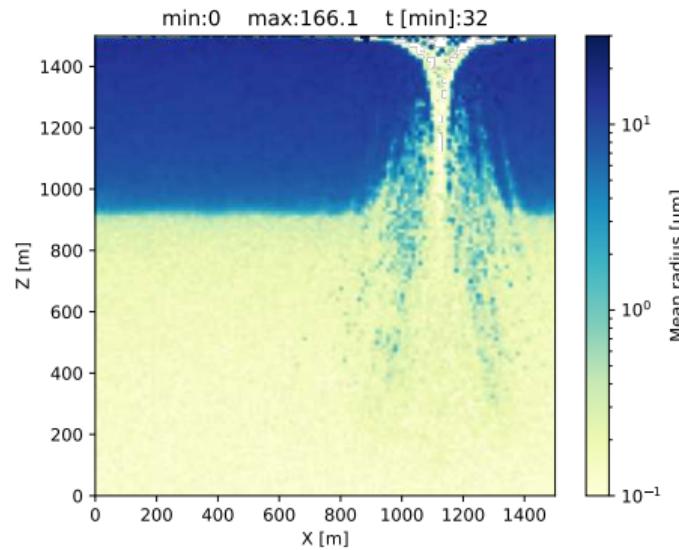
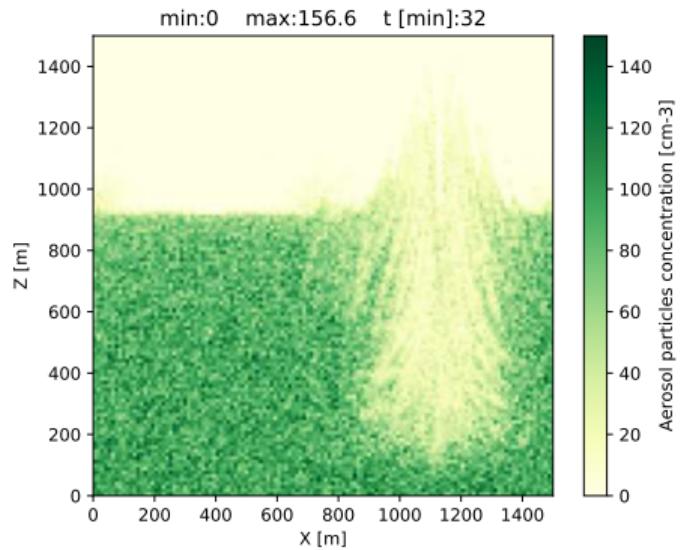
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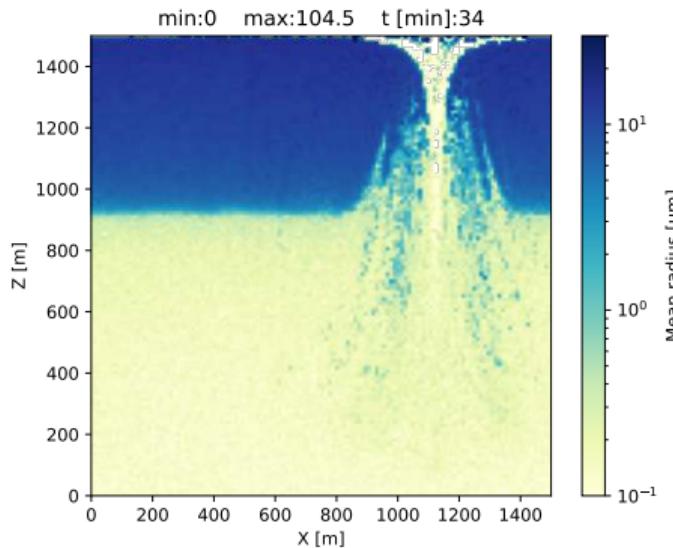
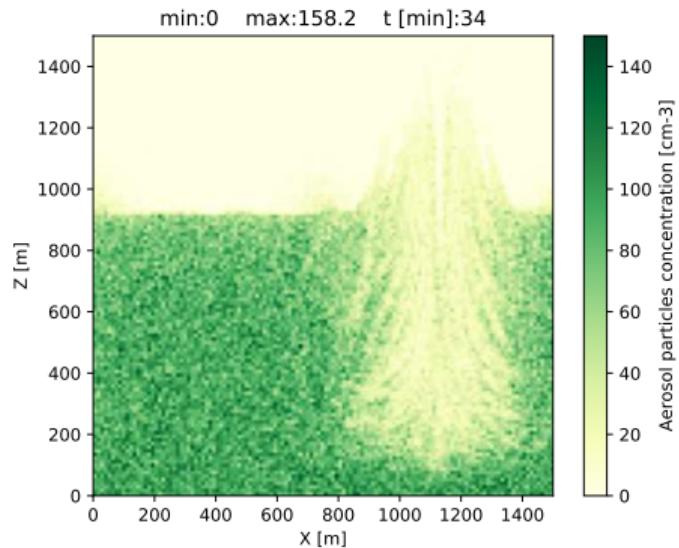
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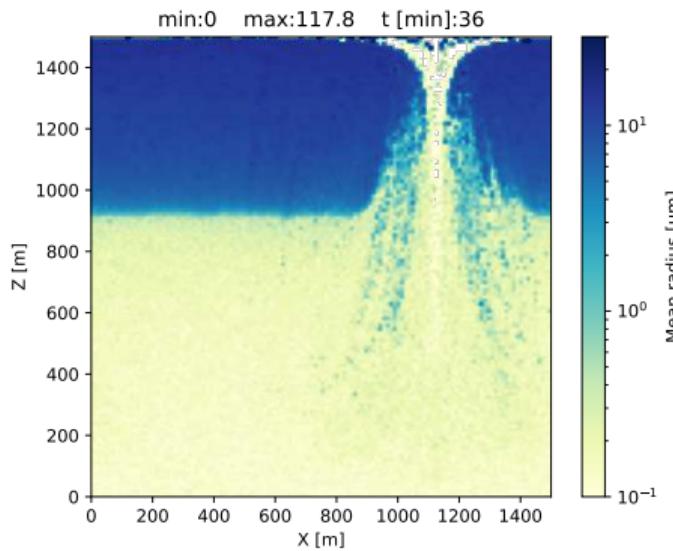
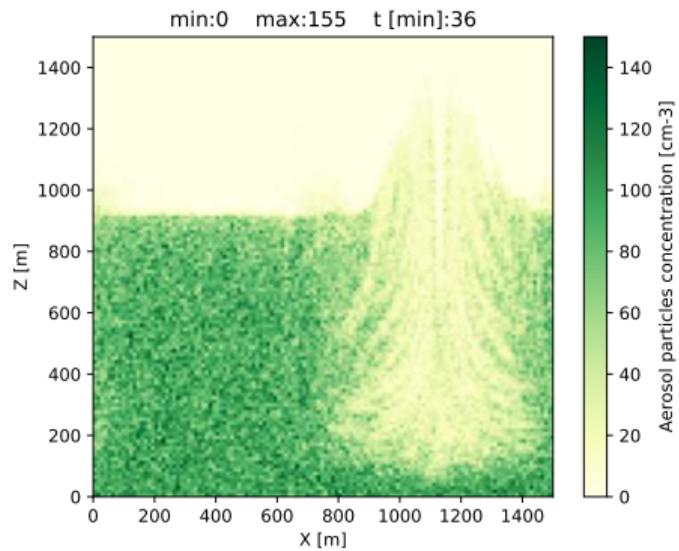
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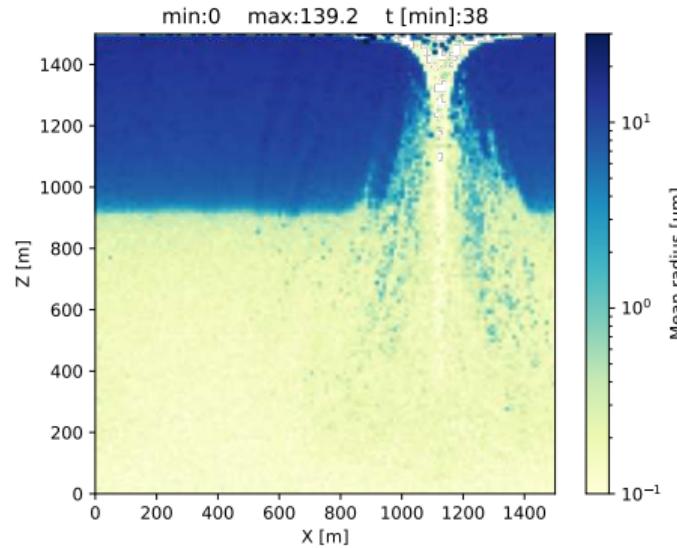
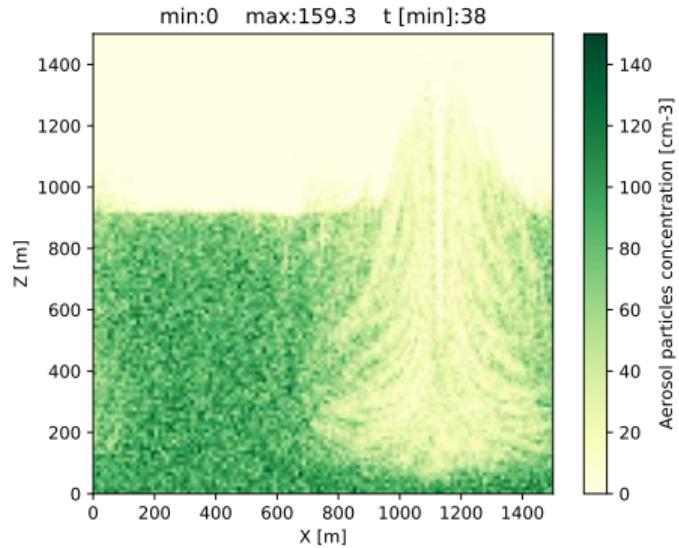
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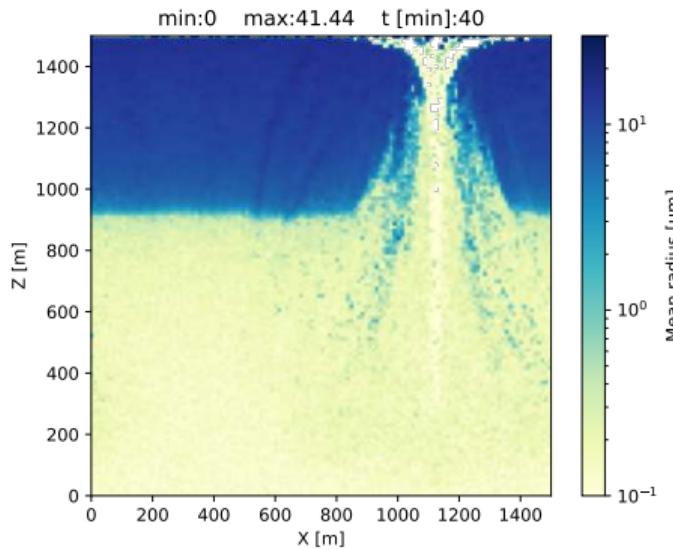
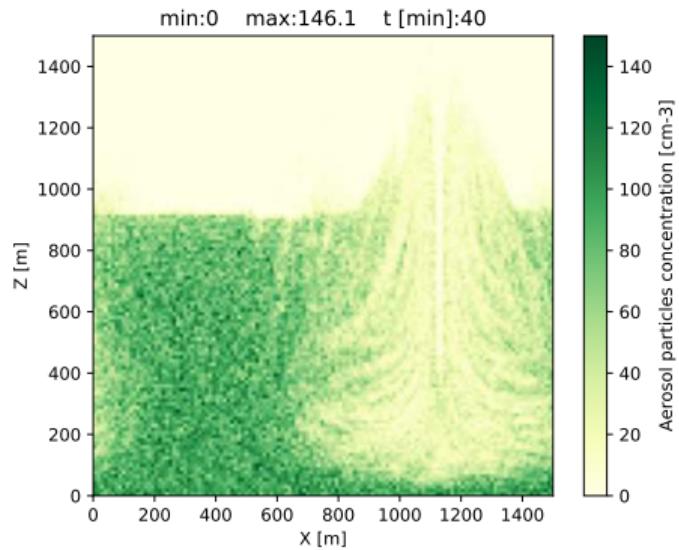
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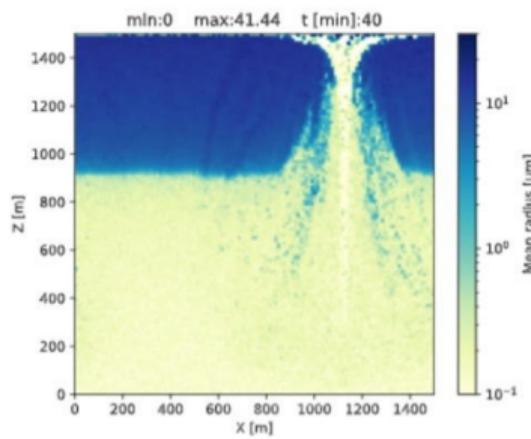
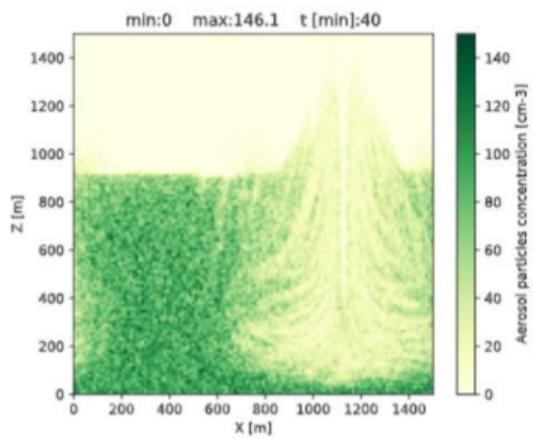


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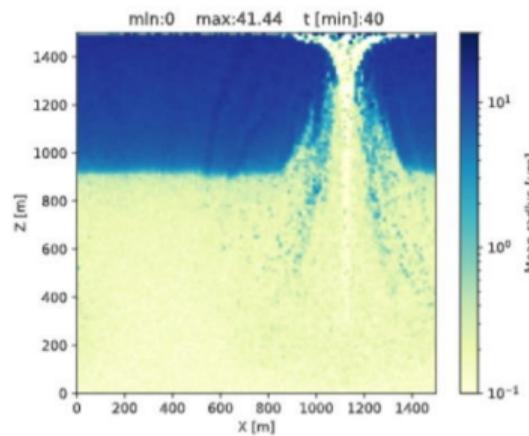
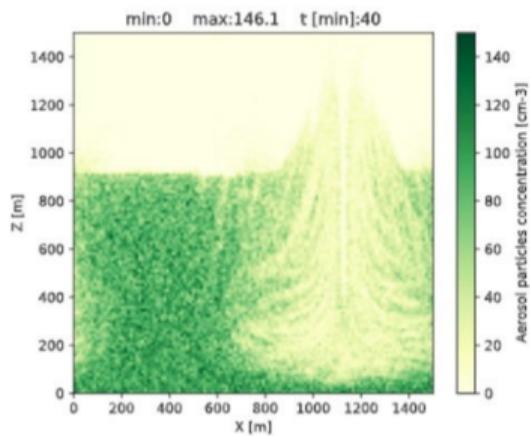
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simulation & vis.: Piotr Bartman



```
[3] 1 simulation.run()
```





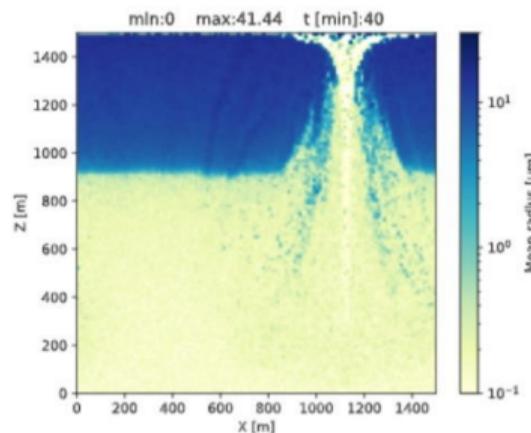
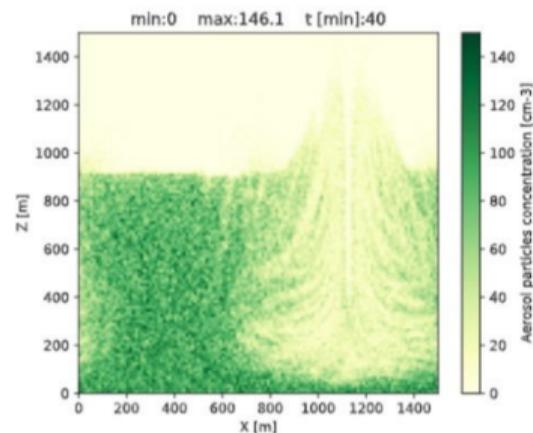
+ Code + Text

RAM
Disk

Editing



[3] 1 simulation.run()



demo.ipynb

File Edit View Insert Runtime Tools Help All changes saved

Comment Share P

+ Code + Text

RAM Disk Editing

[3] 1 simulation.run()

Q

<>

□

min:0 max:146.1 t [min]

Z [m]

X [m]

Aerosol

44 t [min]:40

10¹

10⁰

10⁻¹

Mean radius [μm]

Notebook settings

Hardware accelerator

GPU

To get the most out of Colab, avoid using a GPU unless you need one. [Learn more](#)

Omit code cell output when saving this notebook

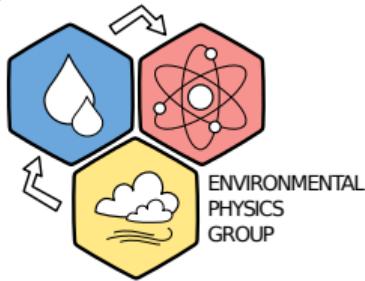
CANCEL SAVE

9/26

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								
Gedzelman & Arnold 1994			x					#dynamics
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
de Jong et al. 2023		x		x				#analytic-solution
...								
OD parcel environment								
Rozanski & Sonntag 1982	x		x					#iterative-parcel
Abdul-Razzak & Ghan 2000	x							#pysdm-vs-gcm-param
Kreidenweis et al. 2003	x				x			#Hoppel-gap
Arabas and Shima 2017	x							#dynamics
Jensen and Nugent 2017	x							#giant-CCN
Yang et al. 2018	x							#ripening
Lowe et al. 2019	x							#surfactants
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...								
1D single-column kinematic env. (advection: PyMPDATA)								
Shipway & Hill 2012	x	x			x			#KiD
deJong et al. 2023 (figures 6-8)	x	x		x	x			#KiD
...								
2D prescribed-flow environment (advection: PyMPDATA)								
Arabas et al. 2015	x	x			x			#GUI
Arabas et al. 2023 (figure 11)	x	x			x	x		#Paraview





■ 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

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- ▶ IAEA/GNIP site in Kraków
- ▶ 50-year precip isotopic data record
- ▶ high-altitude lab (clouds in-situ)
@Kasprowy Wierch (1987 m AMSL)

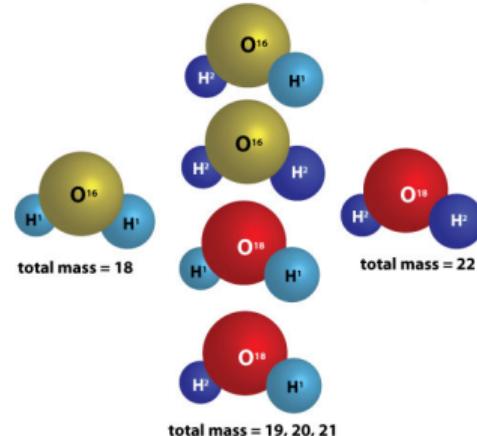


photo: naukaoklimacie.pl

clouds from a water isotopic point of view

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

Oxygen and hydrogen isotopes in water
Light $\xrightarrow{\hspace{1cm}}$ Heavy

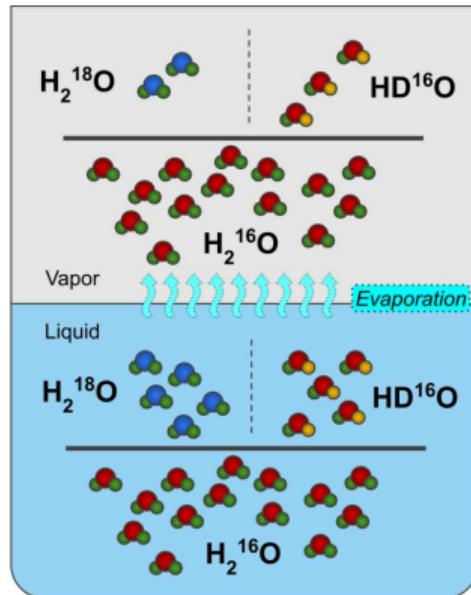


graphic: usgs.gov

$$M_v \approx 18.015 \text{ g/mol}$$

clouds from a water isotopic point of view

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

$$\alpha_{\text{eq}}^{\text{HDO}}(20^\circ\text{C}) = e_s^{\text{light}} / e_s^{\text{heavy}} \approx 1.08$$

$$\alpha_{\text{eq}}^{\text{H}_2^{18}\text{O}}(20^\circ\text{C}) \approx 1.01$$

clouds from a water isotopic point of view

- ☒ water isotopologues (stable): H_2O (99.7%), H_2^{18}O (0.2%), HDO (0.03%), H_2^{17}O (0.04%), ...
- ☒ condensation “favors” heavy over light isotopologues (evaporation vice versa)
 - ~~ equilibrium fractionation
 - ~~ more pronounced in colder temperatures
 - ~~ larger ($\times 8$) effect for H than O
- ☒ differences in diffusivity in air
 - ~~ non-equilibrium (kinetic) fractionation
 - ~~ applies to sub- and super-saturated conditions
 - ~~ more pronounced for O than H

$$\frac{\alpha_{\text{eff}}}{\alpha_{\text{eq}}} - 1 \approx n \cdot \left(1 - \frac{D^{\text{heavy}}}{D^{\text{light}}}\right) \cdot (1 - \text{RH})$$

α_{eff} effective fractionation coeff.

n turbulence parameter

D diffusion coeffs:

$$\text{HDO: } (1 - D^{\text{heavy}} / D^{\text{light}}) \Big|_{T=20^\circ\text{C}} \approx 2.5\%$$

$$\text{H}_2^{18}\text{O: } (1 - D^{\text{heavy}} / D^{\text{light}}) \Big|_{T=20^\circ\text{C}} \approx 2.9\%$$

RH rel. humidity

precipitating cloud as an isotopic distillation column



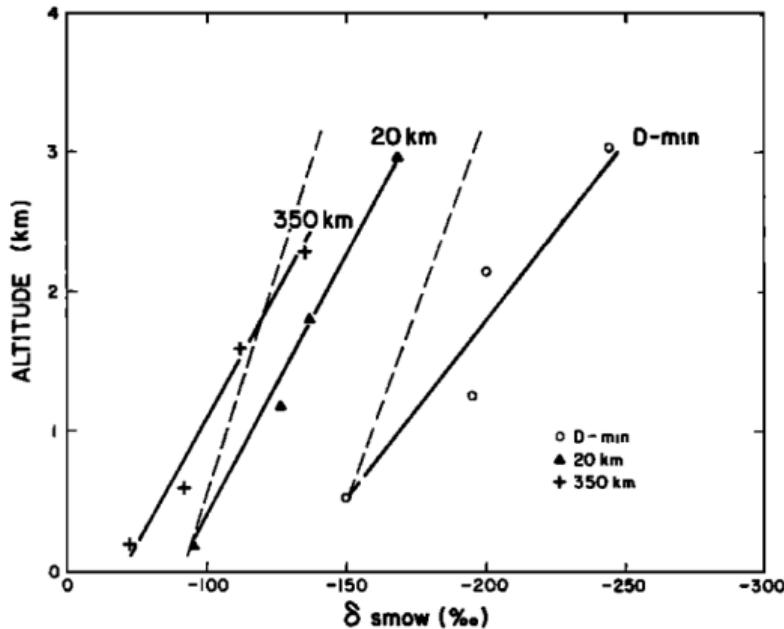
(photo: Yevgen Timashov / National Geographic; Ai-Petri, Crimea, Ukraine)

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Rozanski & Sonntag '82 – iterative parcel PySDM setup

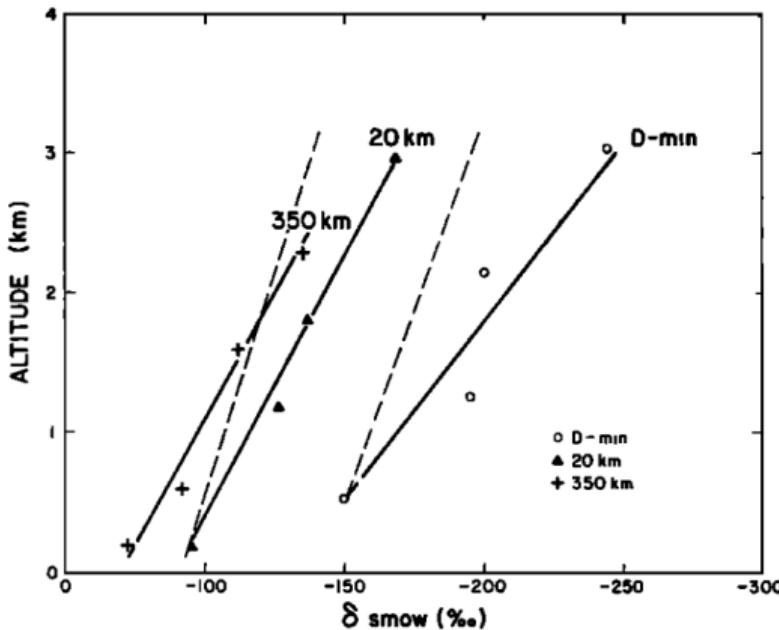
Ehhalt & Östlund 1970



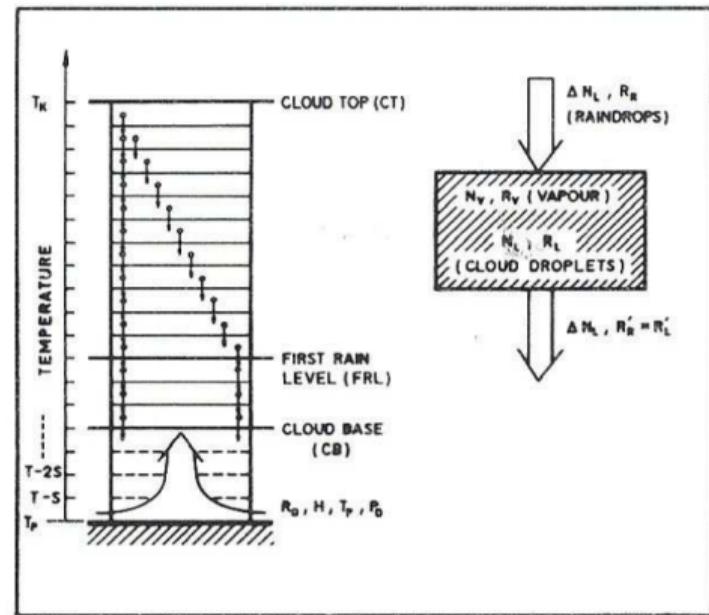
$$\delta_{\text{SMOW}} = \frac{[\text{heavy}]/[\text{light}]|_{\text{sample}}}{[\text{heavy}]/[\text{light}]|_{\text{standard}}} - 1$$

Rozanski & Sonntag '82 – iterative parcel PySDM setup

Ehhalt & Östlund 1970



Rozanski & Sonntag 1982



Rozanski & Sonntag '82 – iterative parcel PySDM setup^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

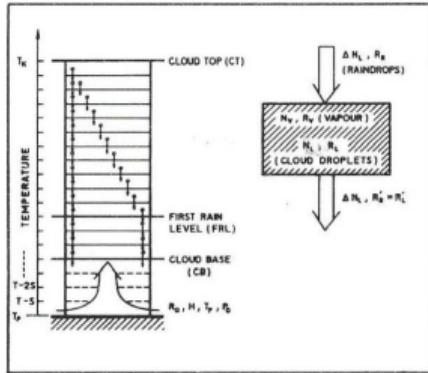


Fig. 3. Schematic diagram of the multibox cloud model.
Input data: initial temperature, T_p ; final temperature, T_k ;
initial pressure, P_0 ; relative humidity, H ; initial isotopic
composition of water vapour, R_0 ; cloud water mixing ratio,
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 K .

Tellus 34 (1982), 2

Rozanski & Sonntag '82 – iterative parcel PySDM setup^a

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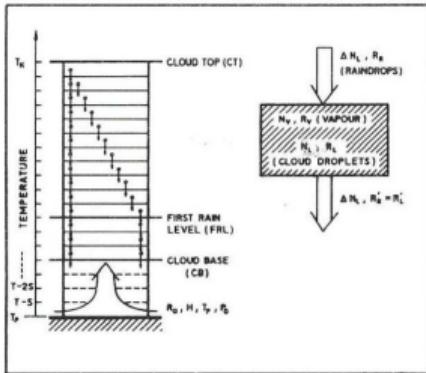


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Tellus 34 (1982), 2

hydrostatic/adiabatic rainshaft with precip removal

Rozanski & Sonntag '82 – iterative parcel PySDM setup^a

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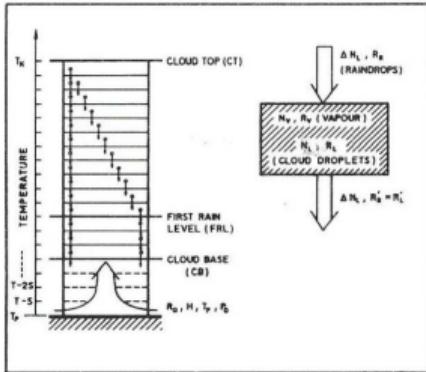


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- hydrostatic/adiabatic rainshaft with precip removal
- condensation: saturation adjustment

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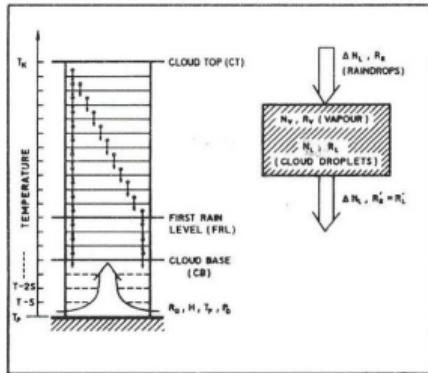


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Tellus 34 (1982), 2

- ▶ hydrostatic/adiabatic rainshaft with precip removal
- ▶ condensation: saturation adjustment
- ▶ rain formation: liquid water content threshold

Rozanski & Sonntag '82 – iterative parcel PySDM setup^a

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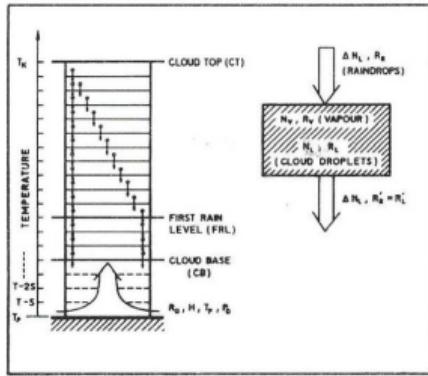


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Tellus 34 (1982), 2

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

Rozanski & Sonntag '82 – iterative parcel PySDM setup^a

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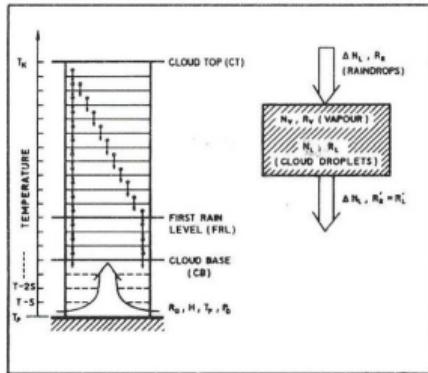


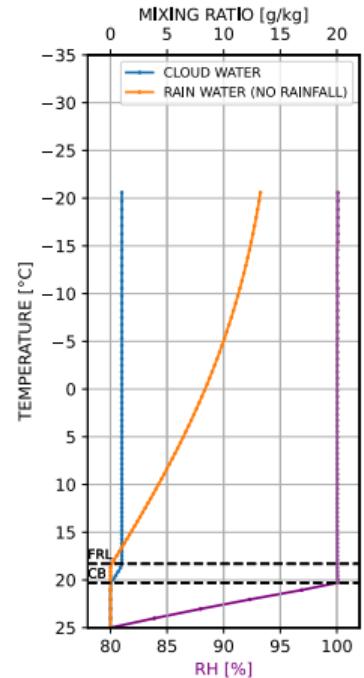
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Tellus 34 (1982), 2

- 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)

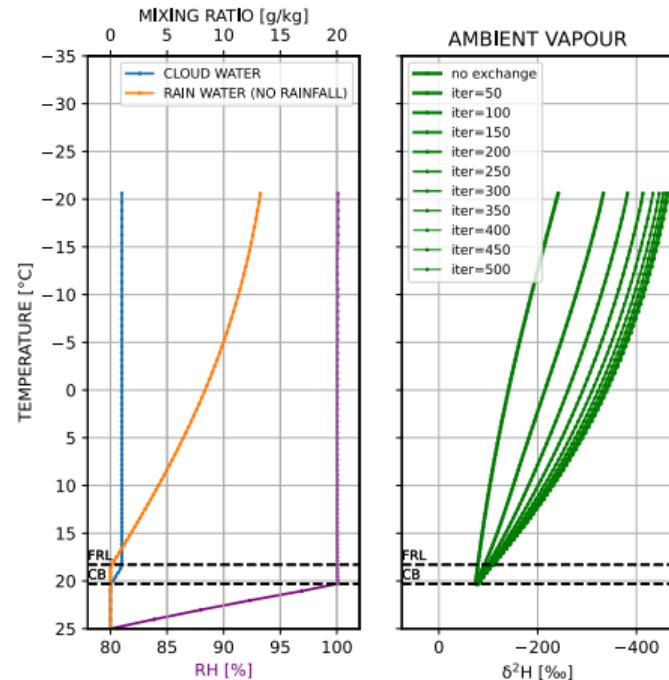
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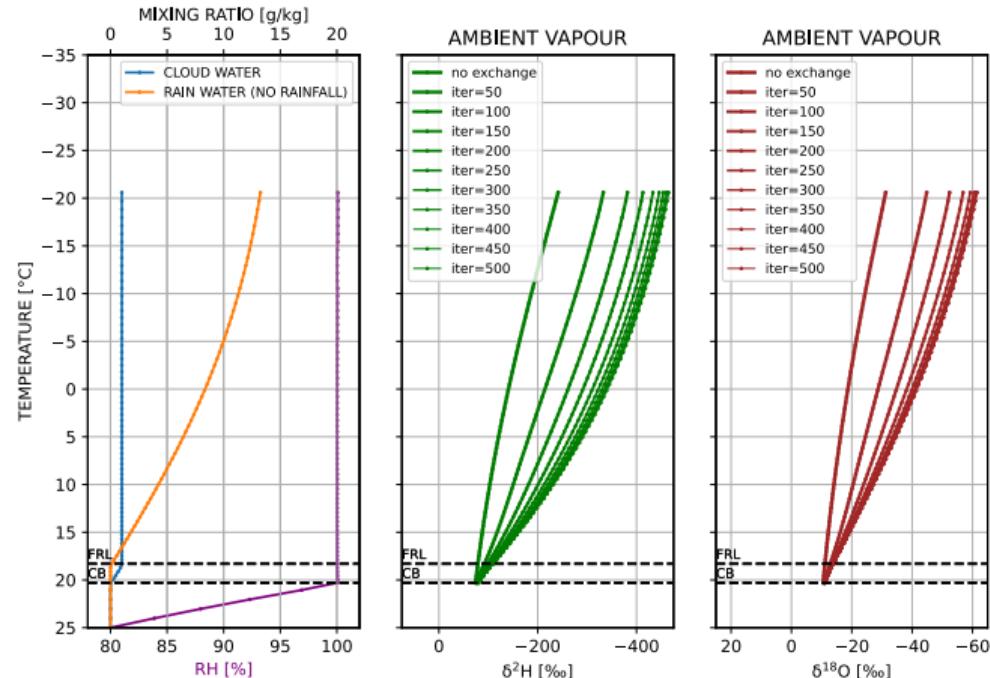
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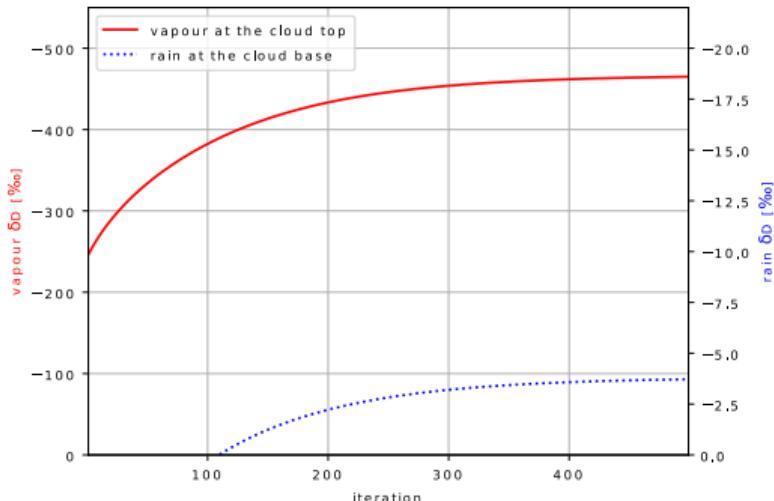
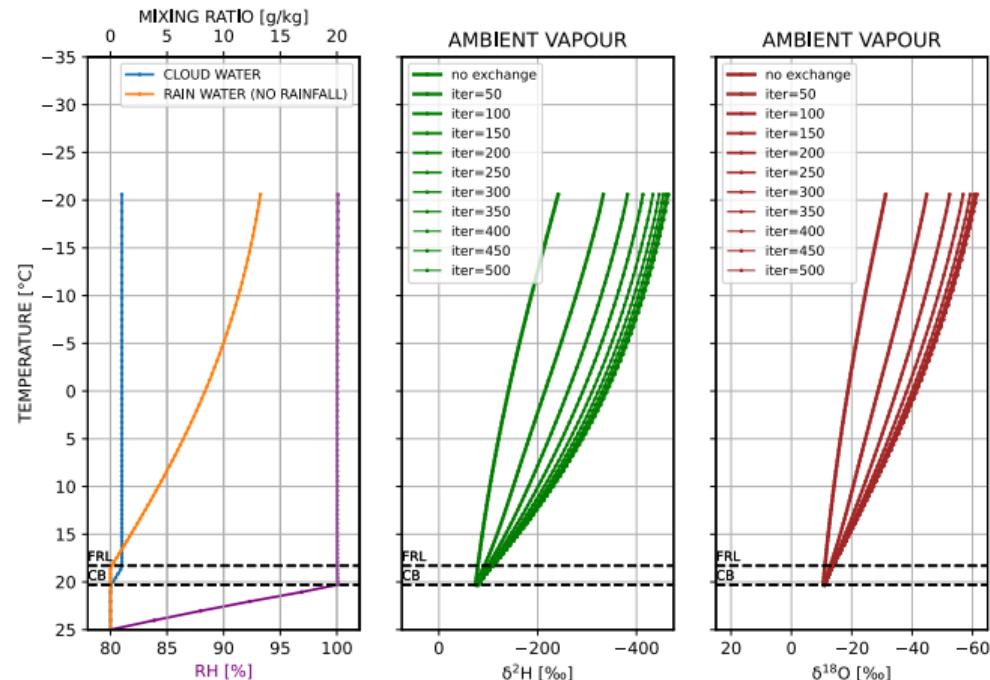
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Shipway & Hill 2012	x	x			x			#KiD
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...								
2D prescribed-flow environment (advection: PyMPDATA)								
Arabas et al. 2015	x	x			x			#GUI
Arabas et al. 2023 (figure 11)	x	x			x	x		#Paraview

^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

doi:10.1016/j.gca.2022.01.020

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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

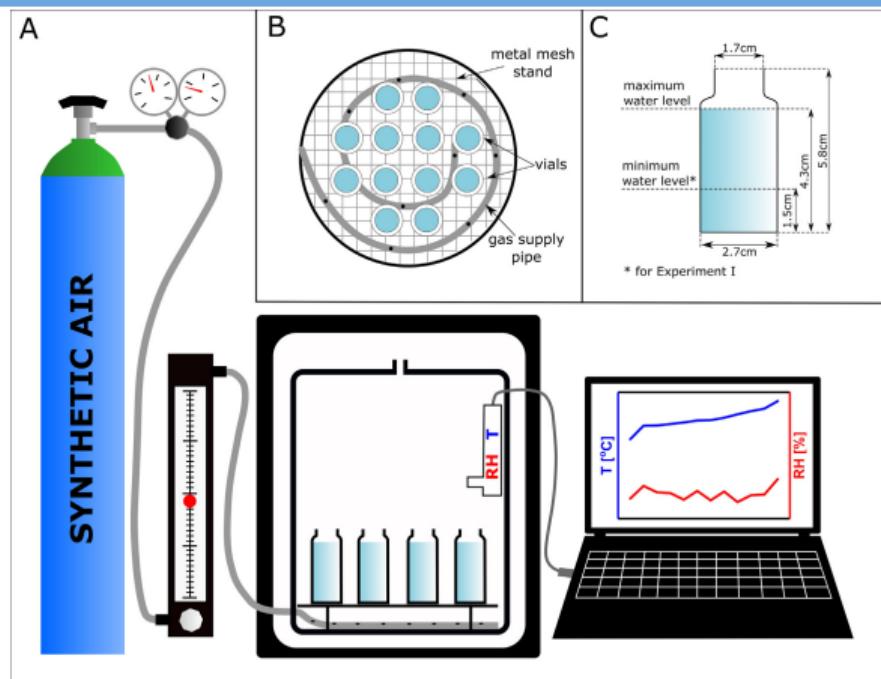
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Received 25 February 2021; accepted in revised form 15 January 2022; Available online 24 January 2022

Pierchala et al. '22 – triple isotope / kinetic fract. PySDM setup^a

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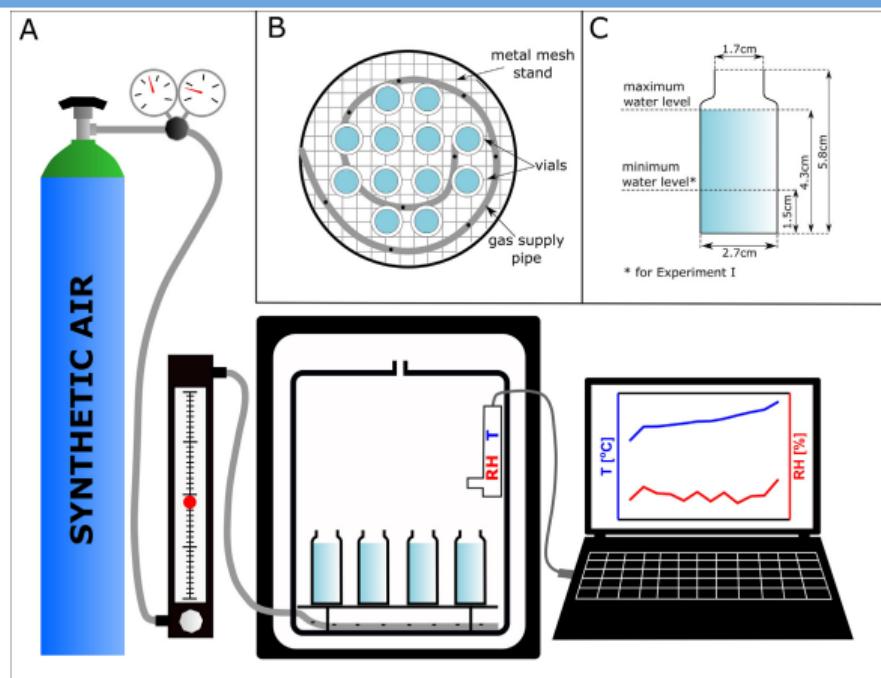
Fig. 1 (paper): lab experiment setup



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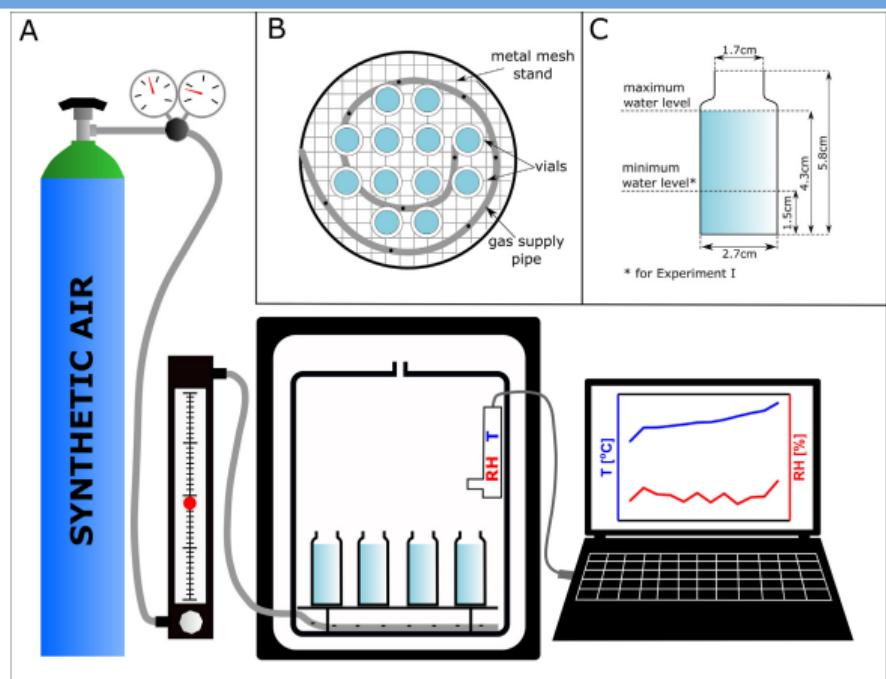


- fractionation upon evaporation (incl. kinetic effects)

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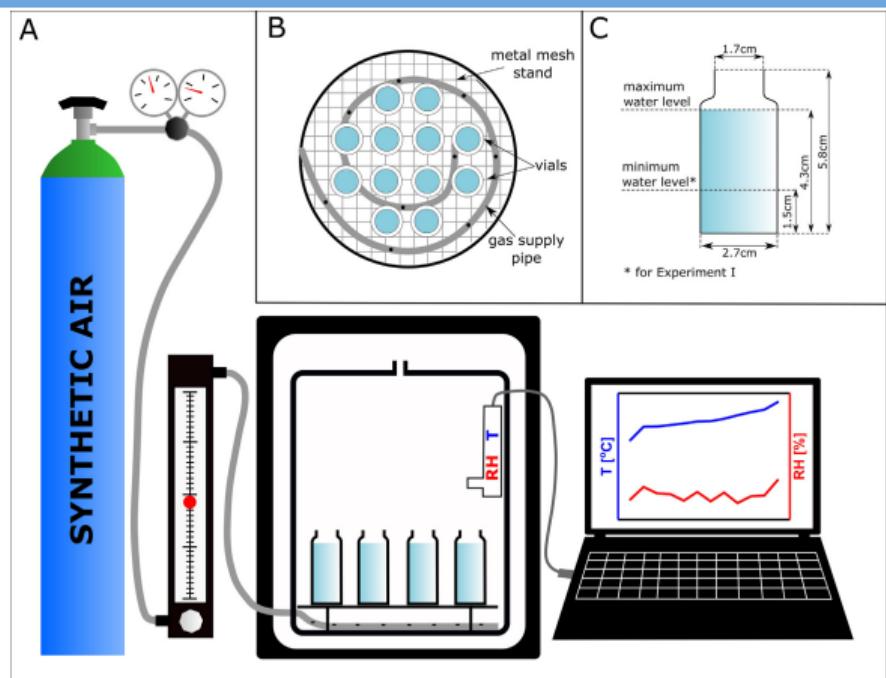


- ❖ fractionation upon evaporation (incl. kinetic effects)
- ❖ multi-day experiments (up to two weeks)

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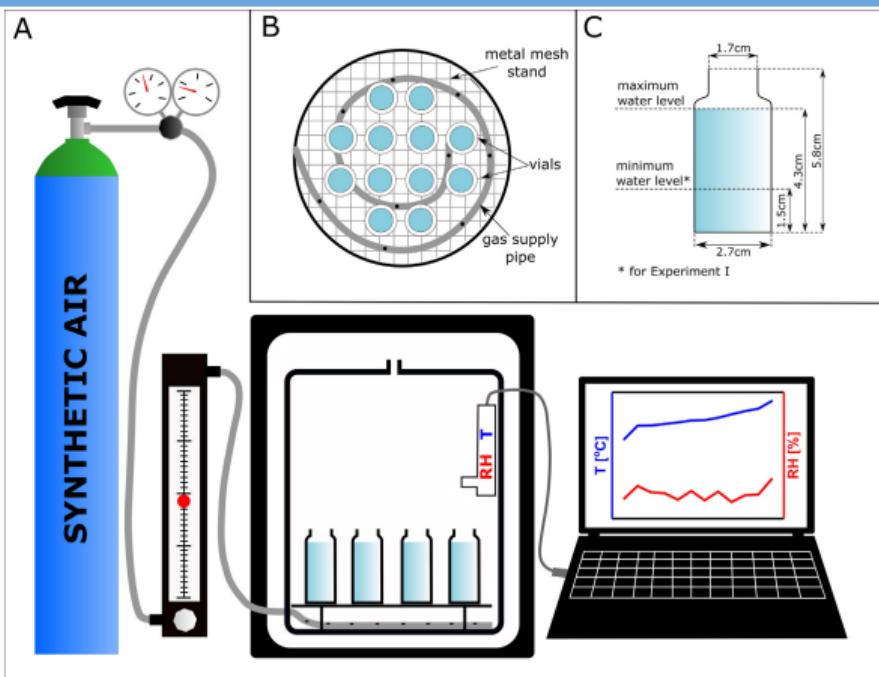


- fractionation upon evaporation (incl. kinetic effects)
- multi-day experiments (up to two weeks)
- Picarro L2140-i cavity ring-down laser spectrometer @AGH (D , ^{18}O , ^{17}O) (probing vaporized water)

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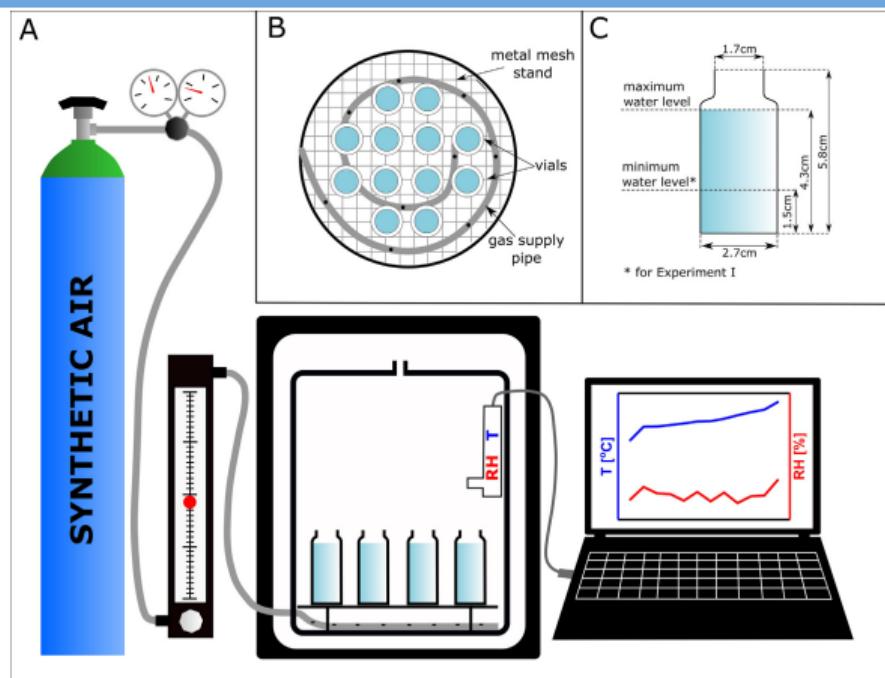


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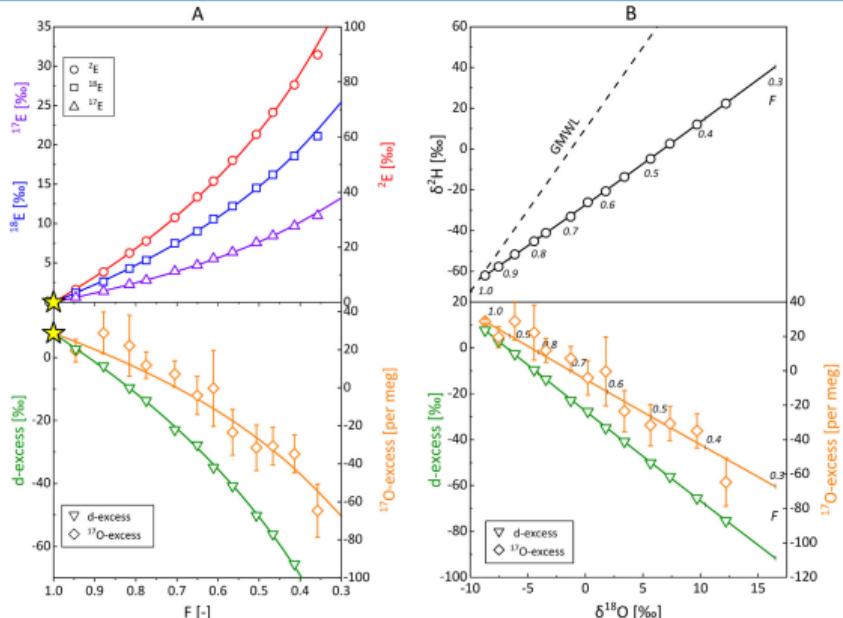


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Fig. 3 (paper): measurements + model



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

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

F: fraction of water remaining

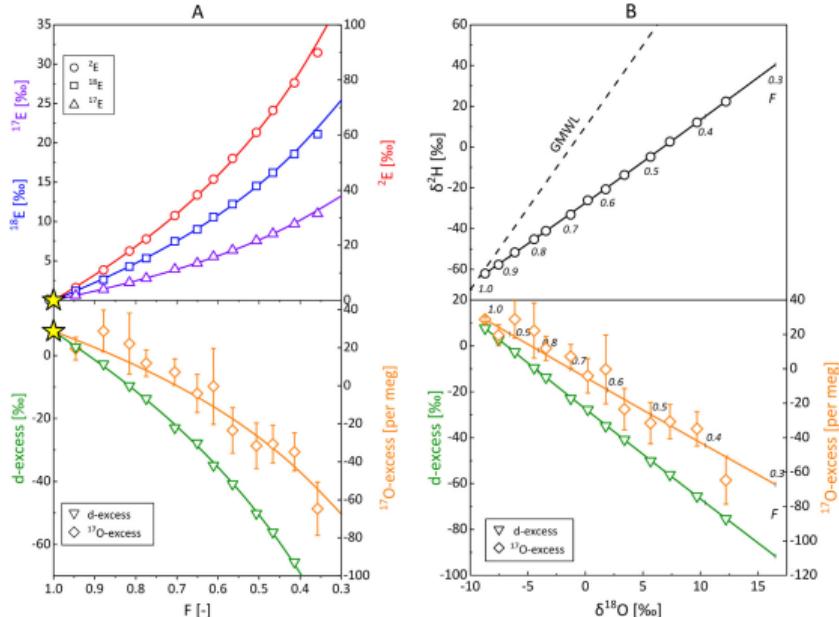
$$d\text{-excess: } \delta^{2}\text{H} - 8 \cdot \delta^{18}\text{O}$$

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

Pierchala et al. '22 – triple isotope / kinetic fract. PySDM setup^a

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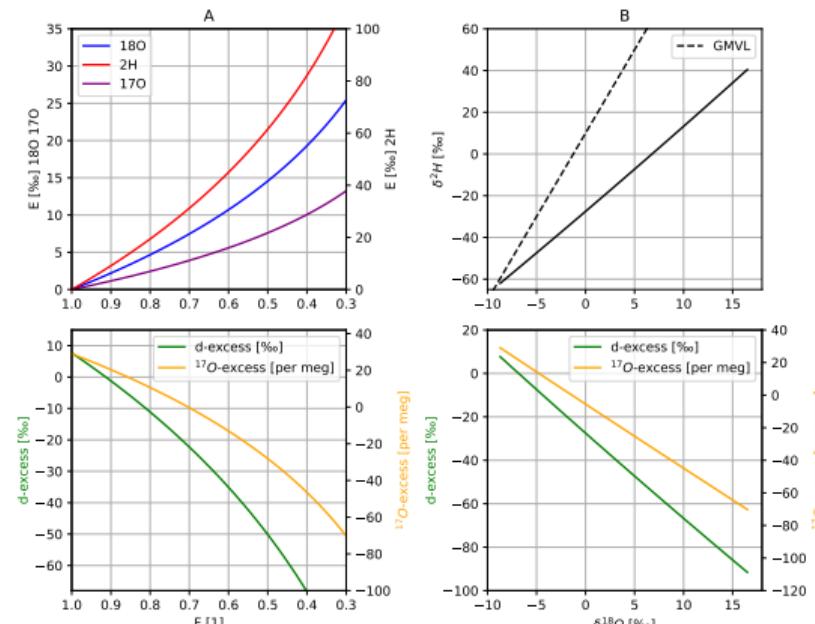
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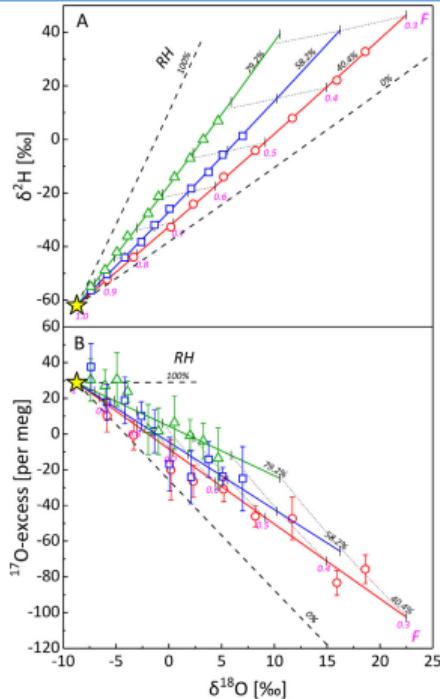
PySDM: theoretical curves



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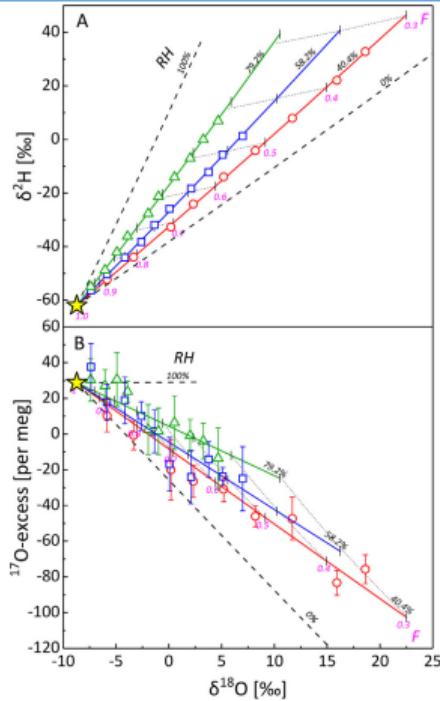
Fig. 4 (paper): RH varied



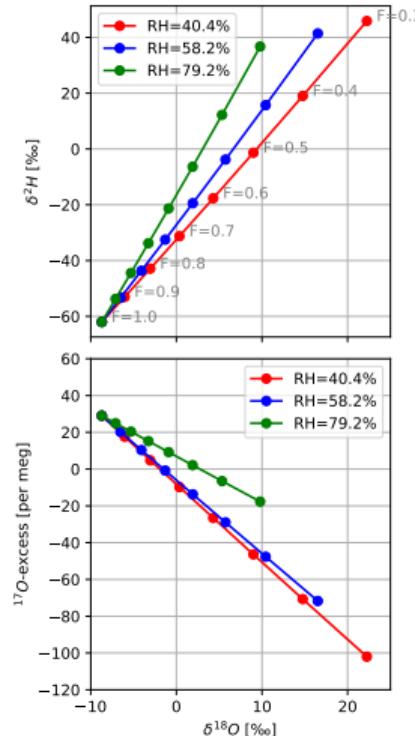
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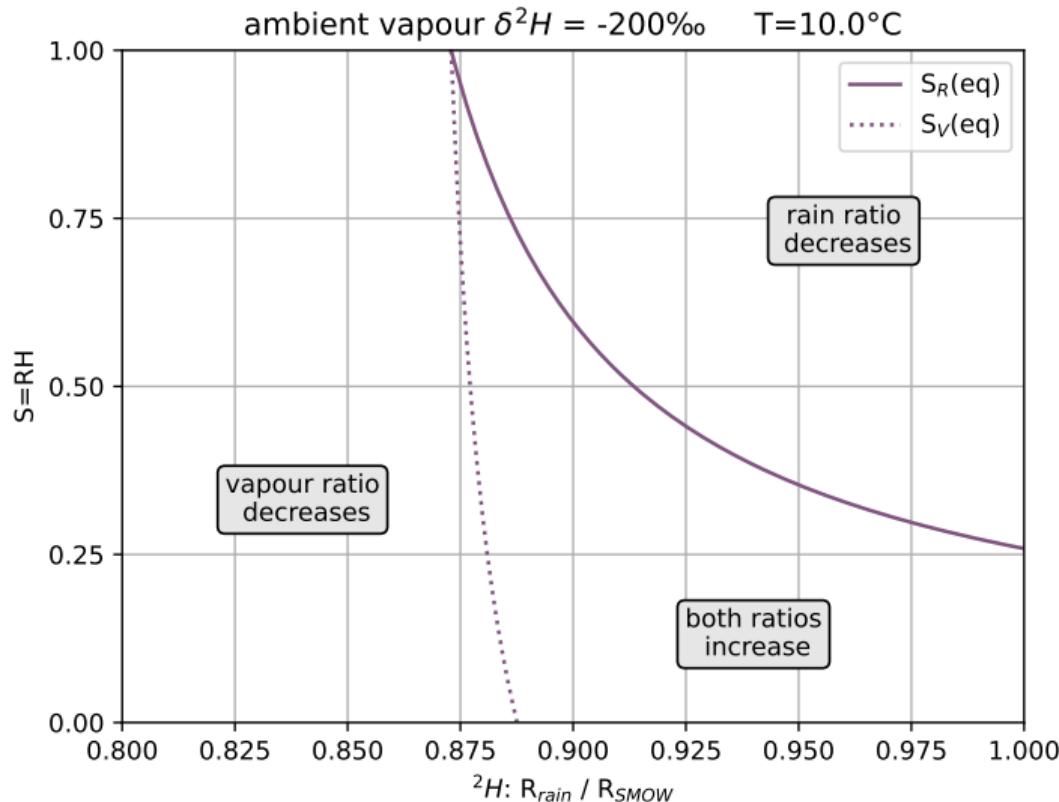
PySDM: model curves



literature reference	cond/evap	coalescence	isotopes	breakup	transport	chemistry	freezing	keywords
formulae-only								
Gedzelman & Arnold 1994			x					#dyncs
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
de Jong et al. 2023	x		x					#analytic-solution
...								
OD parcel environment								
Rozanski & Sonntag 1982	x		x					#iterative-parcel
Abdul-Razzak & Ghan 2000	x							#pysdm-vs-gcm-param
Kreidenweis et al. 2003	x				x			#Hoppel-gap
Arabas and Shima 2017	x							#dyncs
Jensen and Nugent 2017	x							#giant-CCN
Yang et al. 2018	x							#ripening
Lowe et al. 2019	x							#surfactants
Grabowski and Pawlowska 2023	x							#ripening
...								
1D single-column kinematic env. (advection: PyMPDATA)								
Shipway & Hill 2012	x	x			x			#KiD
deJong et al. 2023 (figures 6-8)	x	x		x	x			#KiD
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Arabas et al. 2023 (figure 11)	x	x			x	x		#Paraview

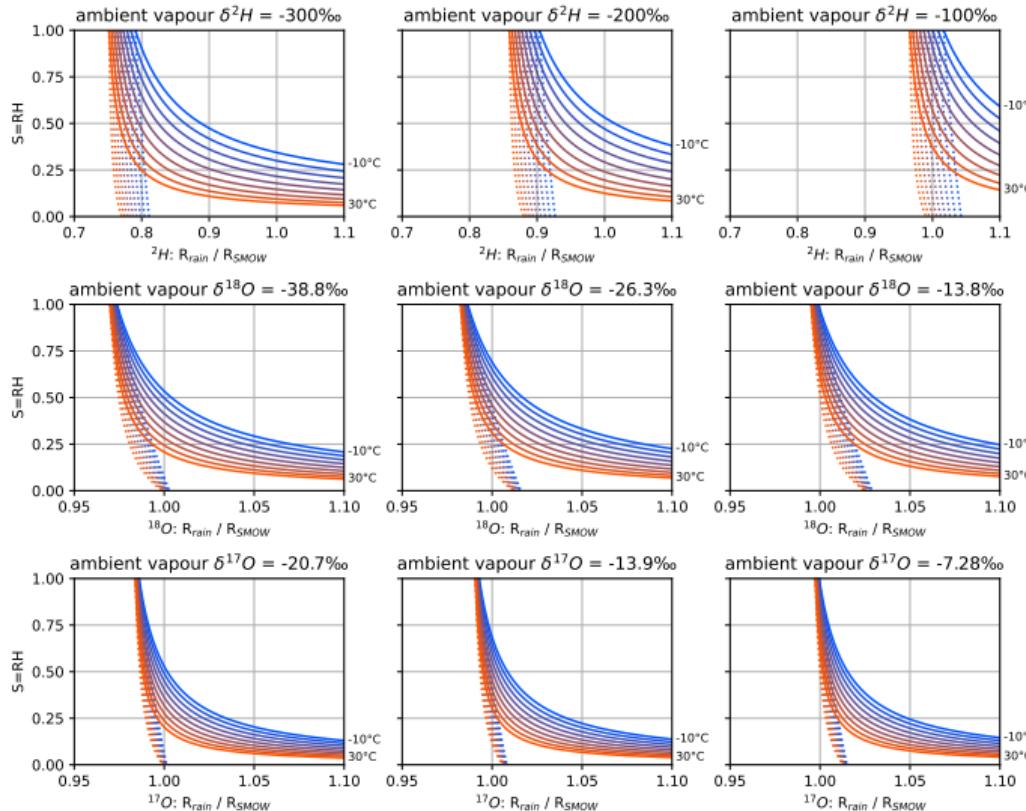
Gedzelman & Arnold 1994: drop evaporation dynamics^a

^ahttps://github.com/open-atmos/PySDM/tree/main/examples/PySDM_examples/Gedzelman_and_Arnold_1994



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water isotopes in PySDM: summary, next steps

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

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- ☒ ice-phase processes

motivation slide!

using water-isotope data to investigate turbulence

Study of Mass Transfer at the Air-Water Interface by an Isotopic Method

L. MERLIVAT

*Departement de Recherche et Analyse, Centre d'Études Nucléaires de Saclay
Gif Sur Yvette, France*

M. COANTIC

Institut de Mécanique Statistique de la Turbulence, Marseille, France

The calculation of the evaporation flux is based on certain assumptions concerning processes in the vicinity of the air-water interface. Most of the recently proposed evaporation theories differ mainly in the estimated contributions of molecular and turbulent mass transfer in the vapor phase just above the liquid surface. This paper will show that, by analyzing the hydrogen and oxygen stable isotope distribution in liquid and water vapor, the processes taking place on a very small scale near the liquid can be investigated. The effect of molecular mass transfer is directly obtained without having to perform difficult measurements in the air in the immediate vicinity of the water surface. Experiments are carried out in the Institut de Mécanique Statistique de la Turbulence air-water tunnel specially designed for the simulation

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supersaturation vs. temperature reconstructions

Theory of isotopic fractionation on faceted ice crystals

J. Nelson

Abstract. The currently used "kinetic-fractionation" (KF) model of the differential incorporation of water-molecule isotopologues into vapor-grown ice omits surface processes on crystal facets that may be important in temperature reconstructions. This article introduces the "surface-kinetic" fractionation model, a model that includes such surface processes, and shows that differences in deposition coefficients for water isotopologues can produce isotopic fractionation coefficients that significantly differ from those of KF theory. For example, if the deposition coefficient of H_2^{18}O differs by just 5% from that of ordinary water (H_2^{16}O), the resulting fractionation coefficient at 20% supersaturation may deviate from the KF value by up to about $\pm 17\%$, and even more at greater supersaturation. As a result, the surface-kinetic theory may significantly change how fractionation depends on supersaturation.

github.com/open-atmos/PySDM

Acknowledgements:

PySDM contributors; prof. Kazimierz Różański (water isotopes)

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merci de votre attention