Modelling of water isotopic fractionation within and below clouds

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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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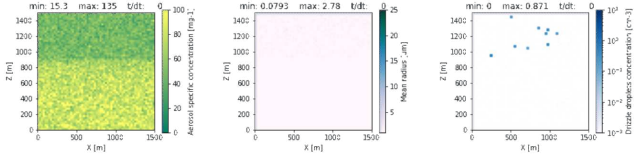

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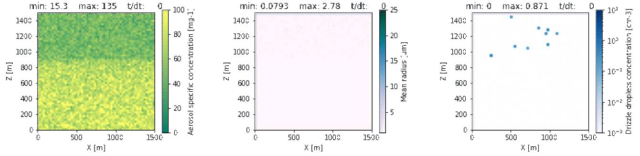

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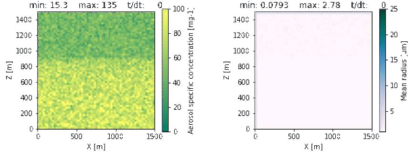

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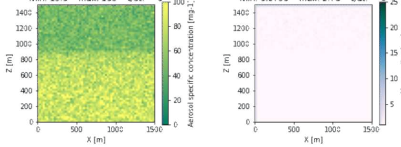

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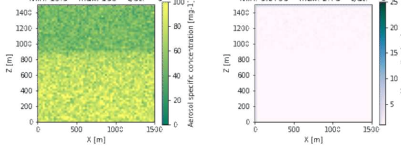

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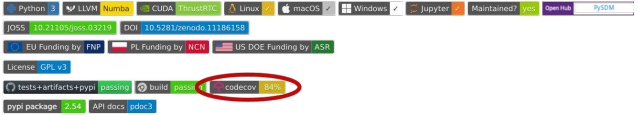

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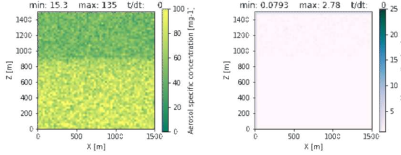

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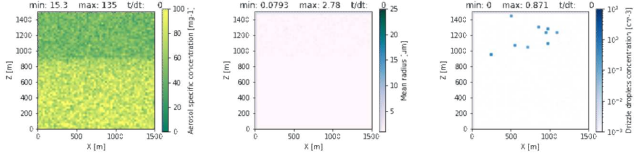

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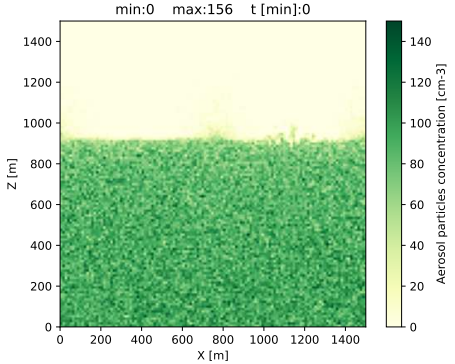
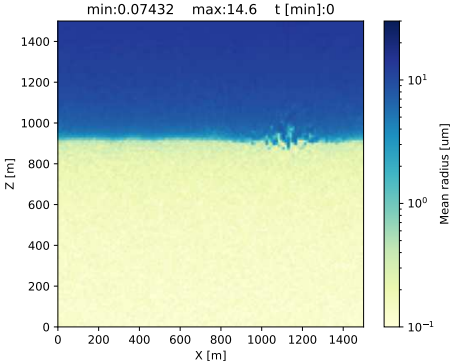
Lagrangian super-particles population: 2^{21}





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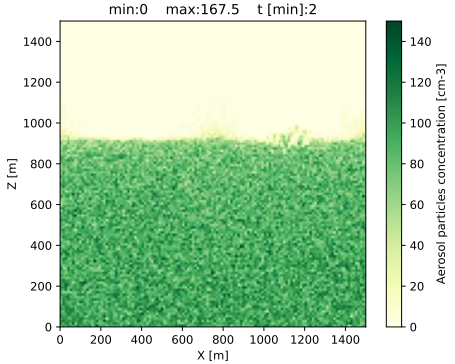

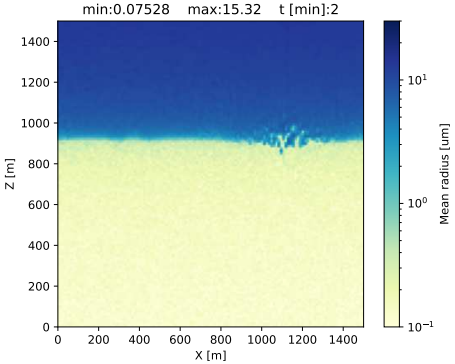

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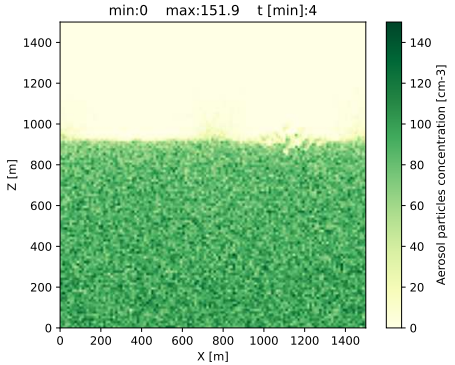

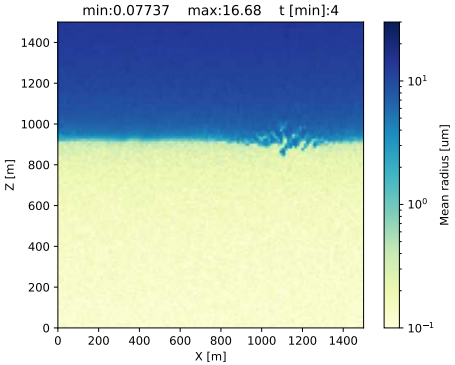

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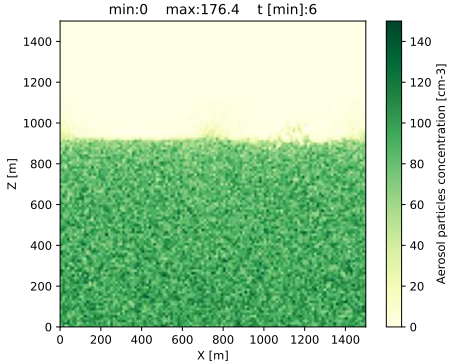

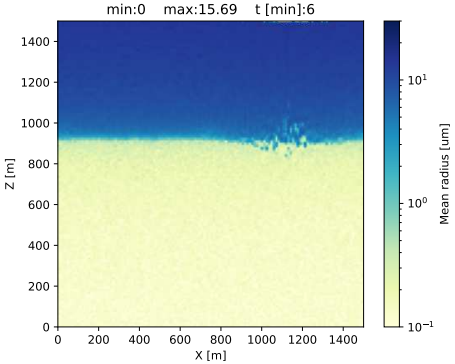

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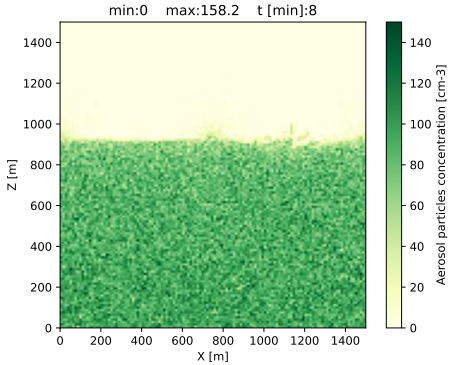

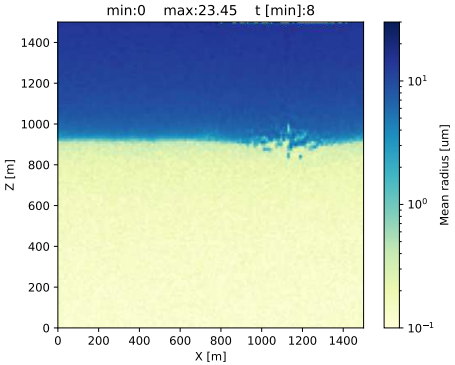

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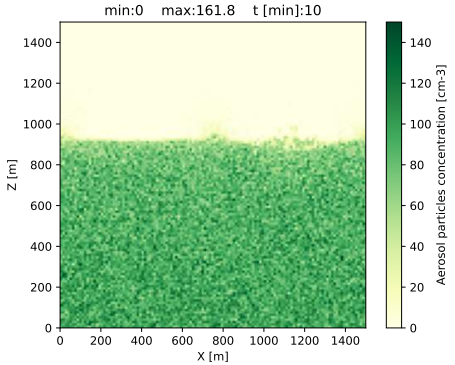

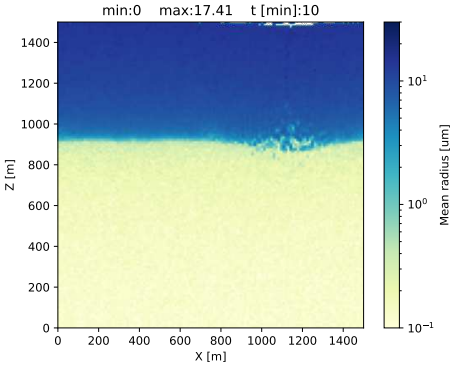

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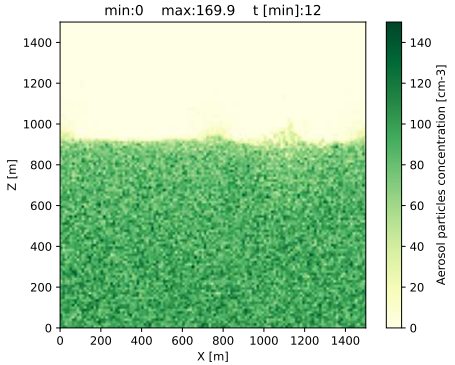

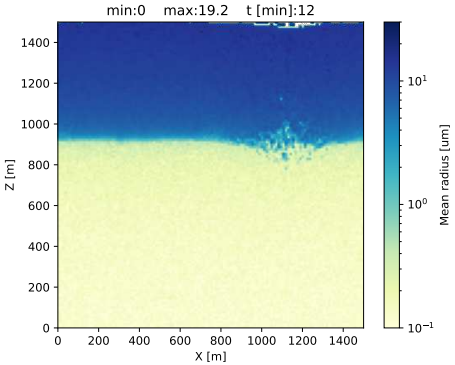

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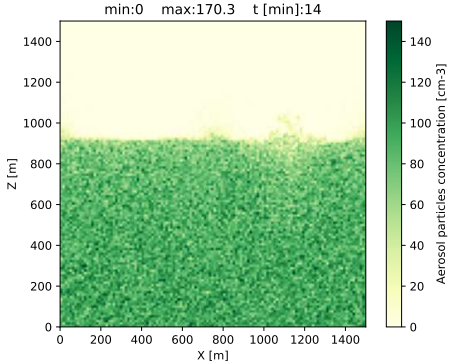

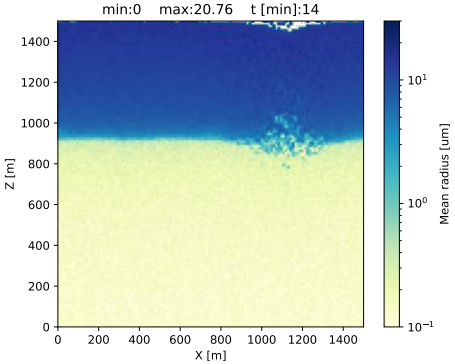

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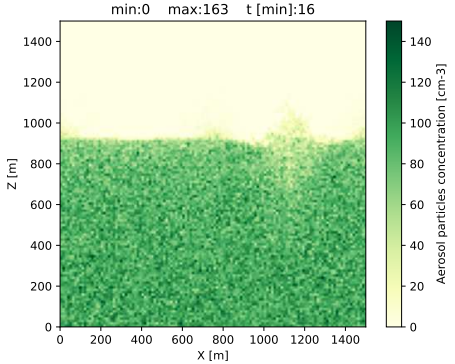

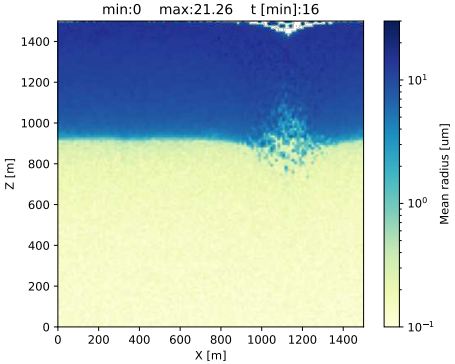

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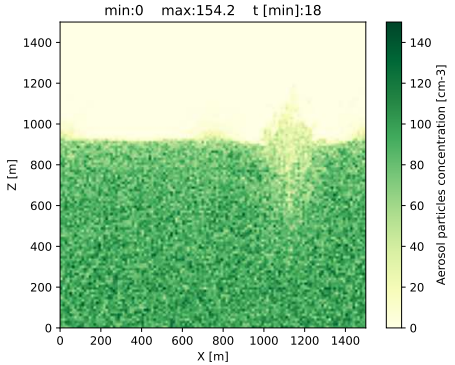
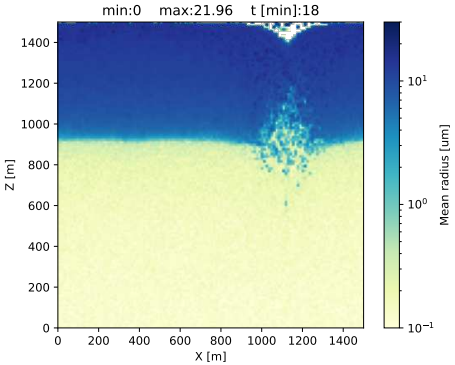
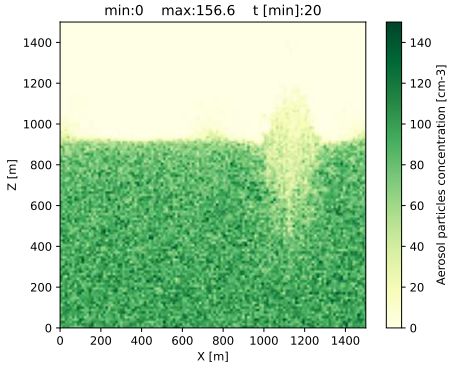
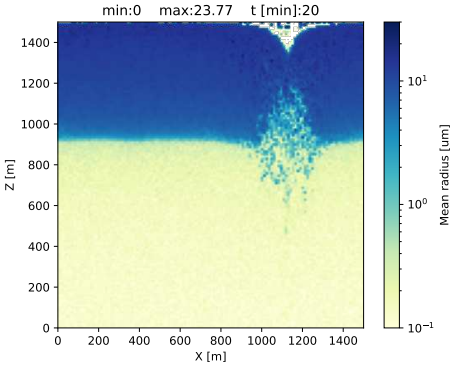




simulation & vis.: Piotr Bartman

Eulerian solver (kinematic flow) grid: 128×128
Lagrangian super-particles population: 2^{21}





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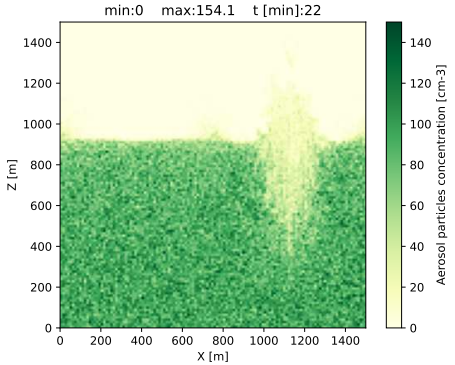

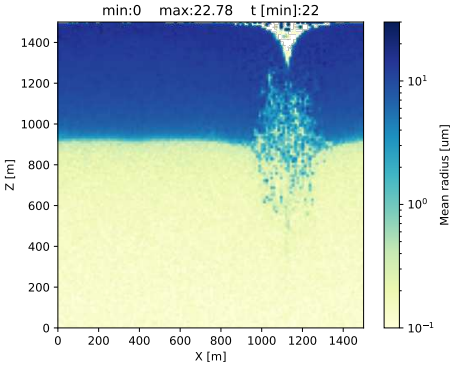

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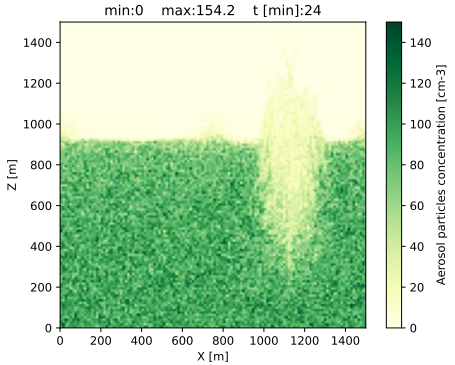

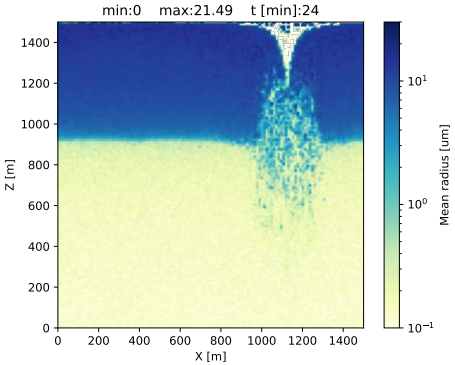

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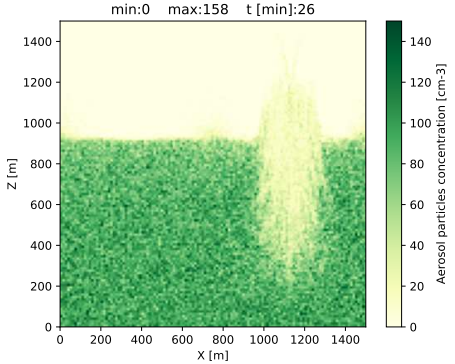

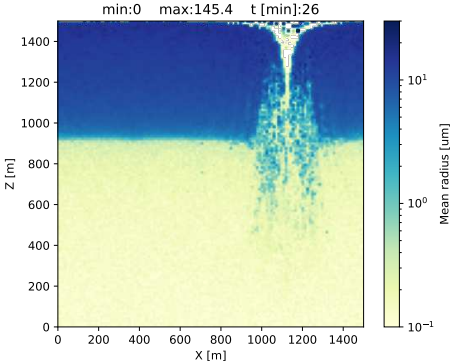

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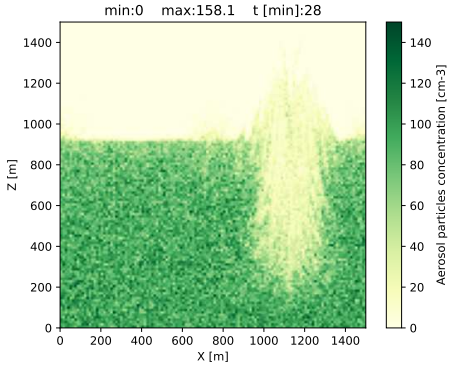

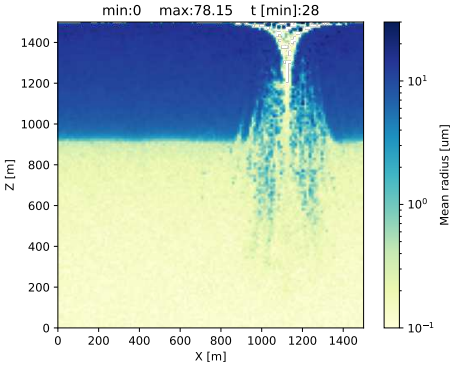

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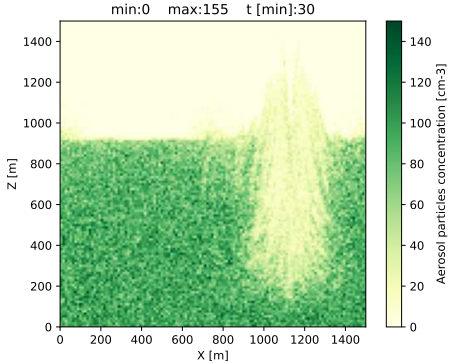

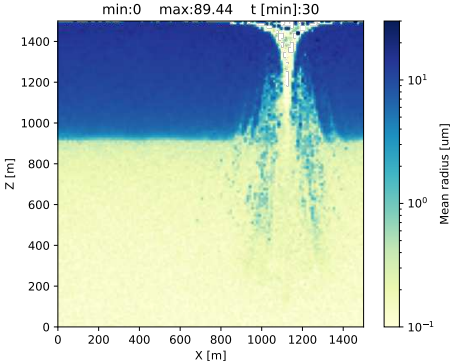

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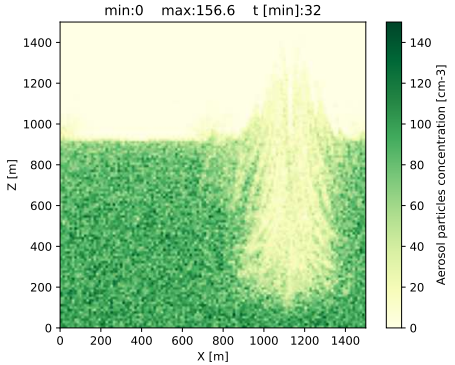

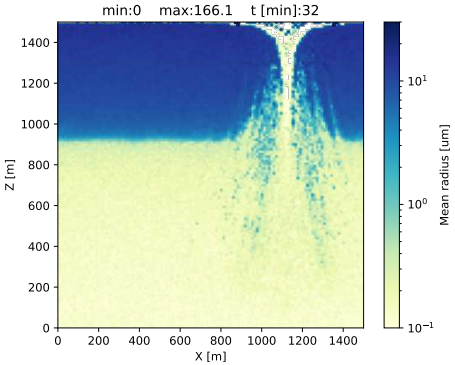

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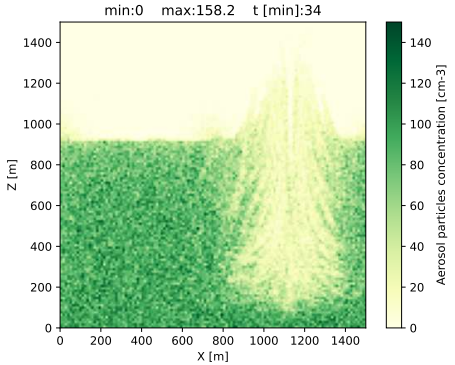

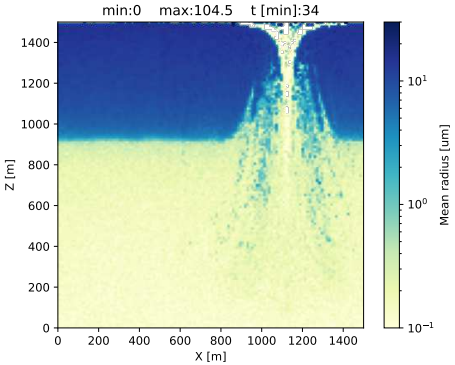

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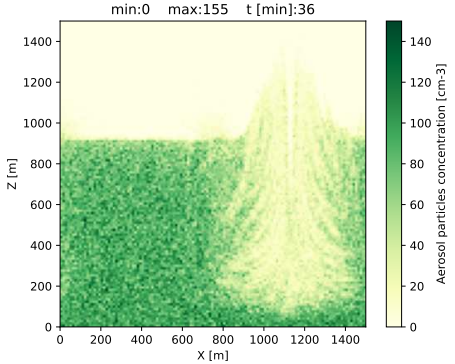

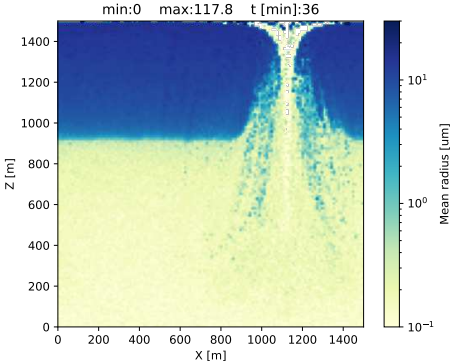

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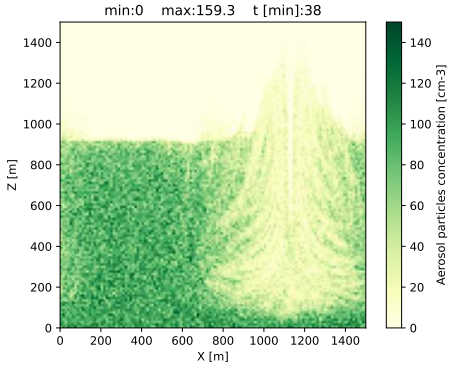

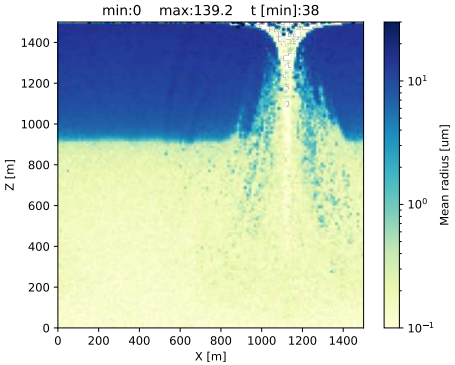

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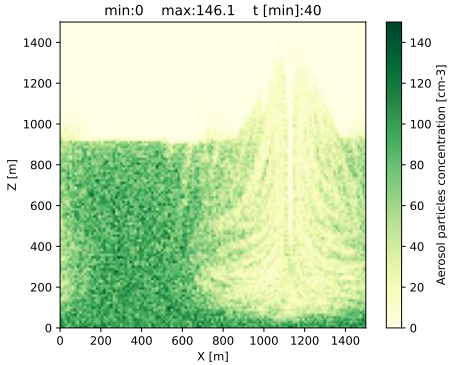
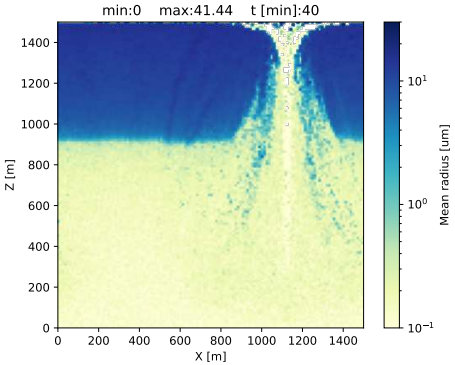
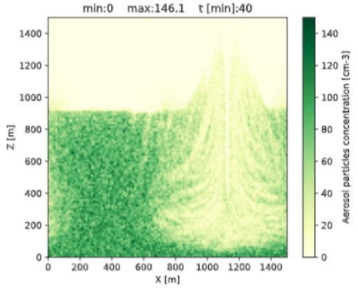
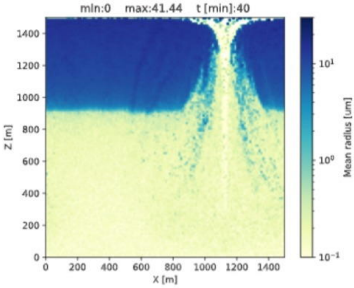


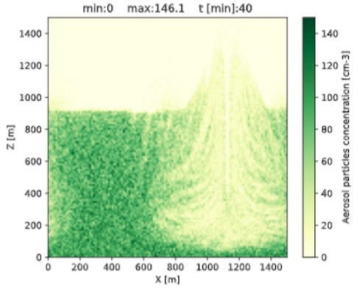


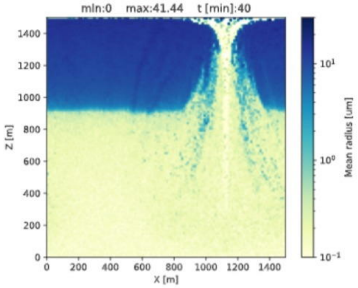
simulation & vis.: Piotr Bartman


min:0 max:146.1 t [min]:40
Z [m]
X [m]
Aerosol particles concentration [cm-3]


min:0 max:41.44 t [min]:40
Z [m]
X [m]
Mean radius [μm]

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





demo.ipynb

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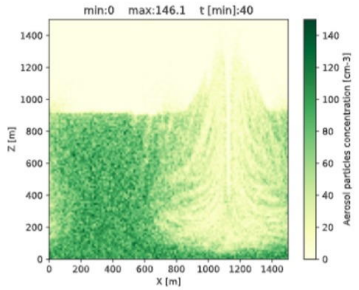
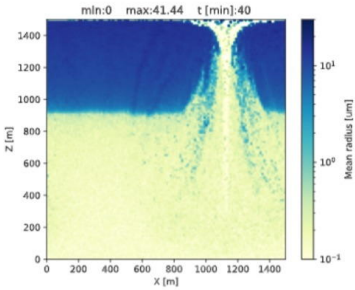
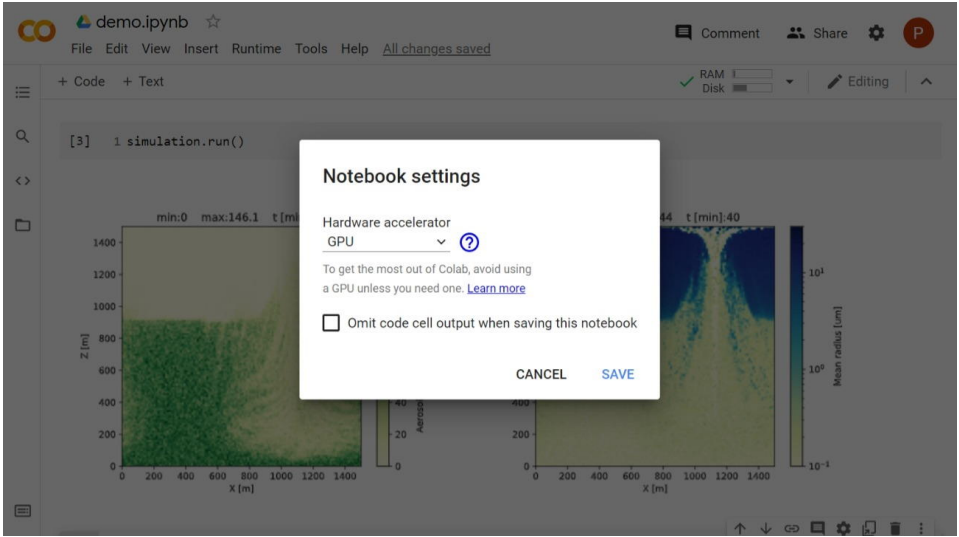
```
[3]  1 simulation.run()
```



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[3] 1 simulation.run()
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
min:0 max:146.1 t [min]:40
Z [m]
X [m]
Mean radius [um]

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								
Gedzelman & Arnold 1994			×					#dynsys
Pierchala et al. 2022			×					#lab-experiment
...								
OD box environment								
Berry 1967		×						#kernels
Shima et al. 2009		×						#analytic-solution
Alpert & Knopf 2016							×	#ABIFM
de Jong et al. 2023		×		×				#analytic-solution
...								
OD parcel environment								
Rozanski & Sonntag 1982	×		×					#iterative-parcel
Abdul-Razzak & Ghan 2000	×							#pysdm-vs-gcm-param
Kreidenweis et al. 2003	×					×		#Hoppel-gap
Arabas and Shima 2017	×							#dynsys
Jensen and Nugent 2017	×							#giant-CCN
Yang et al. 2018	×							#ripening
Lowe et al. 2019	×							#surfactants
Grabowski and Pawlowska 2023	×							#ripening
...								
1D single-column kinematic env. (advection: PyMPDATA)								
Shipway & Hill 2012	×	×			×			#KiD
deJong et al. 2023 (figures 6-8)	×	×		×	×			#KiD
...								
2D prescribed-flow environment (advection: PyMPDATA)								
Arabas et al. 2015	×	×			×			#GUI
Arabas et al. 2023 (figure 11)	×	×			×		×	#Paraview


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ENVIRONMENTAL
PHYSICS
GROUP

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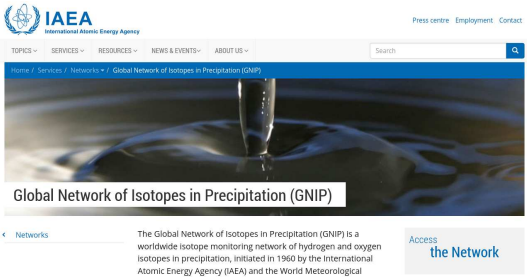
ENVIRONMENTAL
PHYSICS
GROUP



- IAEA/GNIP site in Kraków

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PHYSICS
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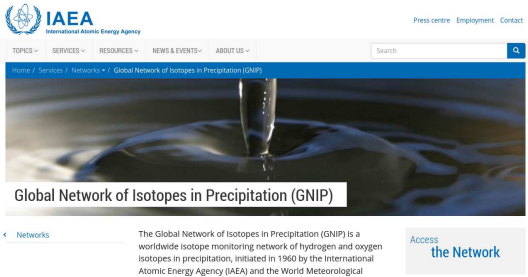

- IAEA/GNIP site in Kraków
- 50-year precip isotopic data record

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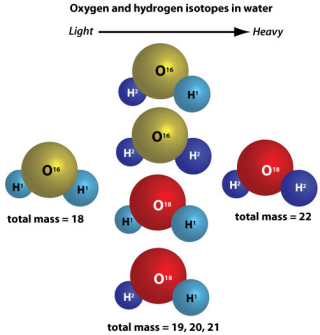
- IAEA/GNIP site in Kraków
- 50-year precip isotopic data record
- high-altitude lab (clouds in-situ)
  @Kasprowy Wierch (1987 m AMSL)

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%), ...



graphic: usgs.gov

$M_v \approx 18.015$ g/mol

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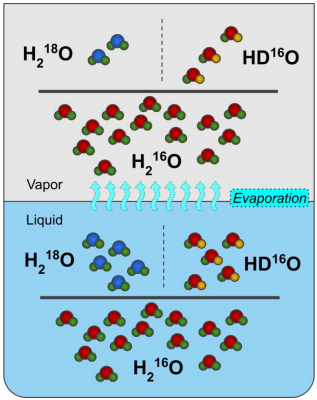
- condensation "favors" heavy over light isotopologues (evaporation vice versa)
  - ⇝ equilibrium fractionation
  - ⇝ more pronounced in colder temperatures
  - ⇝ larger ($\times 8$) effect for H than O



graphic: scisnack.com

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

$$\alpha_{eq}^{H_2^{18}O}(20°C) \approx 1.01$$

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:

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

$H_2{}^{18}O$: $(1 - D^{\text{heavy}}/D^{\text{light}})\big|_{T=20^\circ\text{C}} \approx 2.9\%$

RH rel. humidity

precipitating cloud as an isotopic distillation column

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

clouds from a water isotopic point of view

pypi.org/p/PySDM-examples

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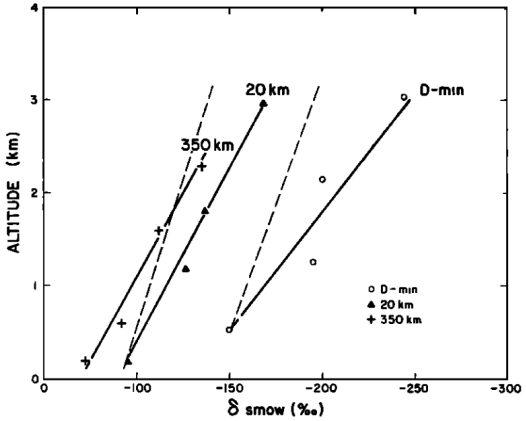
2D prescribed-flow environment (advection: PyMPDATA)								
Arabas et al. 2015	×	×			×			#GUI
Arabas et al. 2023 (figure 11)	×	×			×		×	#Paraview

Rozanski & Sonntag '82 – iterative parcel PySDM setup

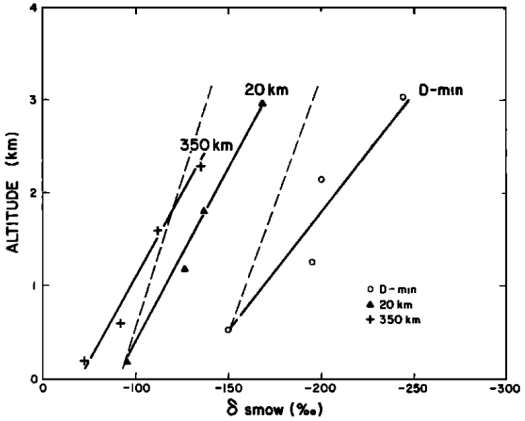
Ehhalt & Östlund 1970



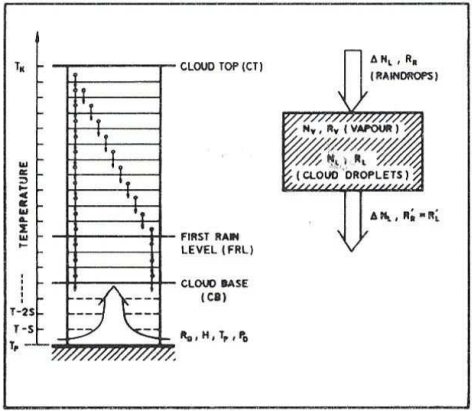
$$\delta_{\text{SMOW}} = \frac{[heavy]/[light]|_{\text{sample}}}{[heavy]/[light]|_{\text{standard}}} - 1$$

Rozanski & Sonntag '82 – iterative parcel PySDM setup

Ehhalt & Östlund 1970



Rozanski & Sonntag 1982



Rozanski & Sonntag '82 – iterative parcel PySDM setup[a]

[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

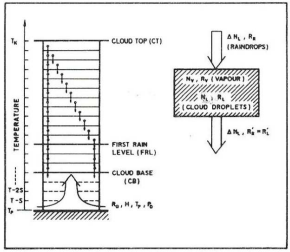


Fig. 3. Schematic diagram of the multibox cloud model. Input data: initial temperature, T_p; final temperature, T_k; initial pressure, P_0; relative humidity, H; initial isotopic composition of water vapour, R_0; cloud water mixing ratio, N_L; temperature step, S; isotope exchange factor, K.

Tellus 34 (1982), 2

Rozanski & Sonntag '82 – iterative parcel PySDM setup[a]

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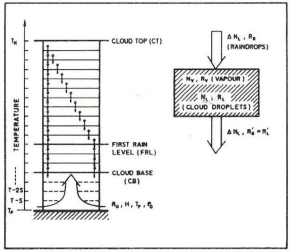

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Tellus 34 (1982), 2

- hydrostatic/adiabatic rainshaft with precip removal

Rozanski & Sonntag '82 – iterative parcel PySDM setup[a]

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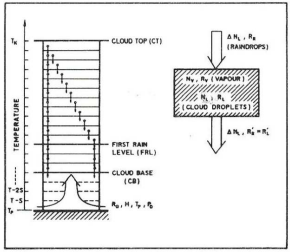

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Tellus 34 (1982), 2

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

Rozanski & Sonntag '82 – iterative parcel PySDM setup[a]

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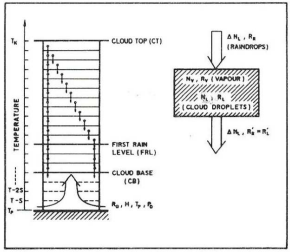

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Tellus 34 (1982), 2

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

Rozanski & Sonntag '82 – iterative parcel PySDM setup[a]

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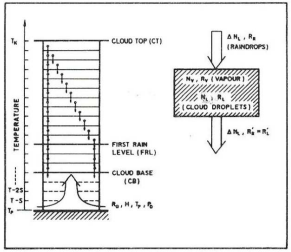

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Tellus 34 (1982), 2

- hydrostatic/adiabatic rainshaft with precip removal
- condensation: saturation adjustment
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- parcel-model iterations towards stationary state (no explicit role of time)

Rozanski & Sonntag '82 – iterative parcel PySDM setup[a]

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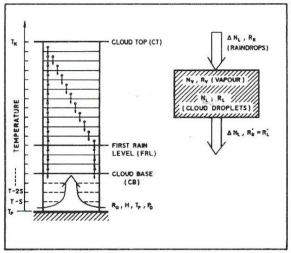

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Tellus 34 (1982), 2

- 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 ($\rightsquigarrow$ hypothesis explaining observed steep $\delta^2\mathrm{H}$ profile gradients beyond condensation-only effects)

Rozanski & Sonntag '82 – iterative parcel PySDM setup[a]

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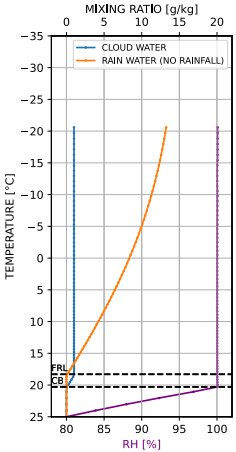

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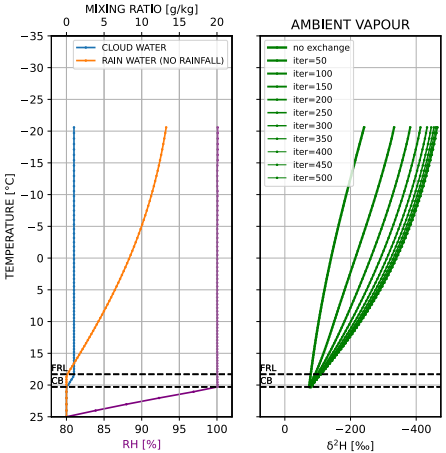

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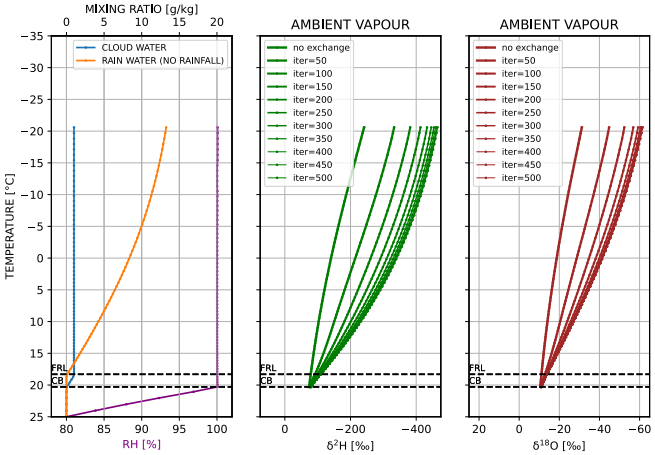

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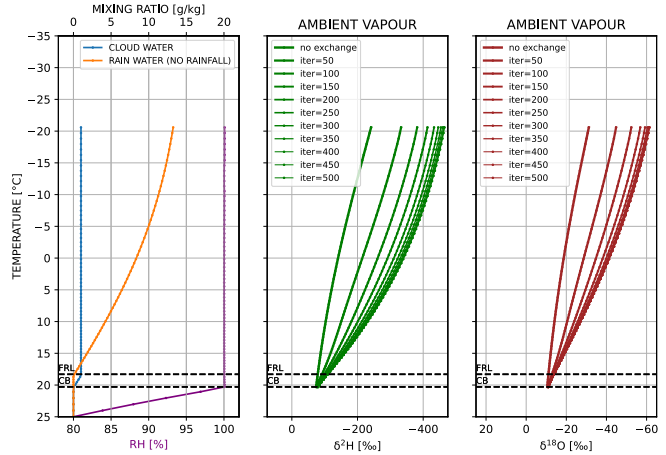

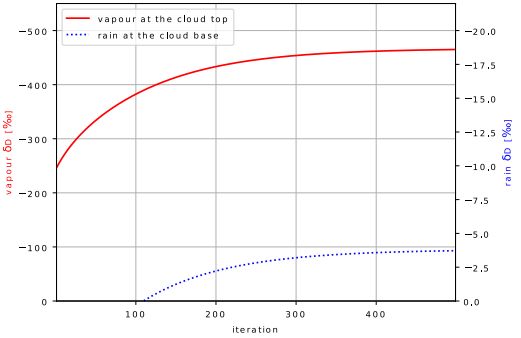

Rozanski & Sonntag '82 – iterative parcel PySDM setup

pypi.org/p/PySDM-examples

literature reference	cond/evap	coalescence	isotopes	breakup	transport	chemistry	freezing	keywords
formulae-only								
Gedzelman & Arnold 1994			×					#dynsys
Pierchala et al. 2022			×					#lab-experiment
...								
OD box environment								
Berry 1967		×						#kernels
Shima et al. 2009		×						#analytic-solution
Alpert & Knopf 2016							×	#ABIFM
de Jong et al. 2023		×		×				#analytic-solution
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OD parcel environment								
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Grabowski and Pawlowska 2023	×							#ripening
...								
1D single-column kinematic env. (advection: PyMPDATA)								
Shipway & Hill 2012	×	×			×			#KiD
deJong et al. 2023 (figures 6-8)	×	×		×	×			#KiD
...								
2D prescribed-flow environment (advection: PyMPDATA)								
Arabas et al. 2015	×	×			×			#GUI
Arabas et al. 2023 (figure 11)	×	×			×		×	#Paraview

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

doi:10.1016/j.gca.2022.01.020

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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

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

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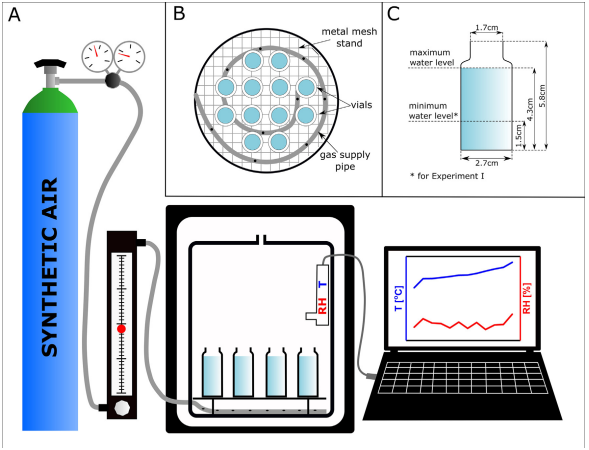
Fig. 1 (paper): lab experiment setup



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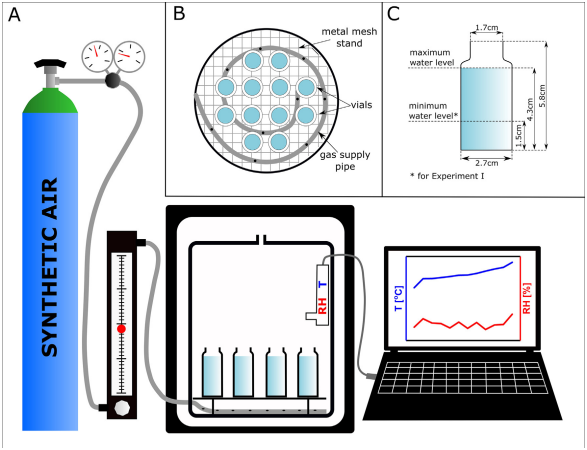

- fractionation upon evaporation (incl. kinetic effects)

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

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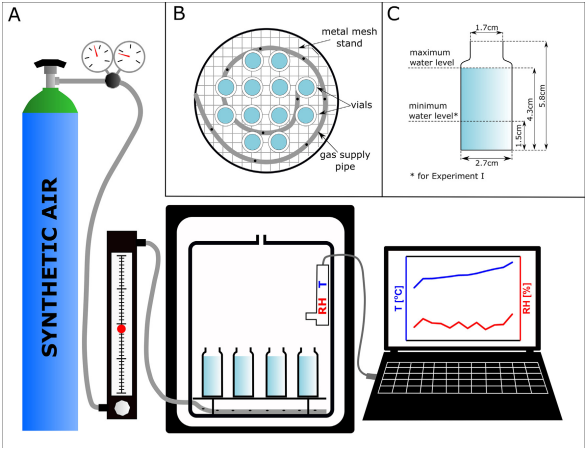

- fractionation upon evaporation (incl. kinetic effects)
- multi-day experiments (up to two weeks)

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

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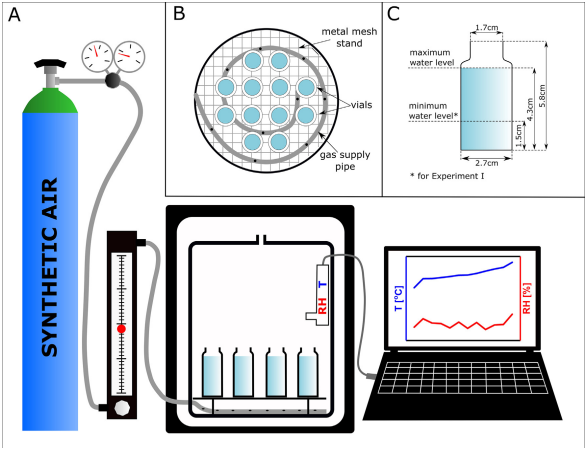

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Pierchala et al. '22 – triple isotope / kinetic fract. PySDM setup[a]

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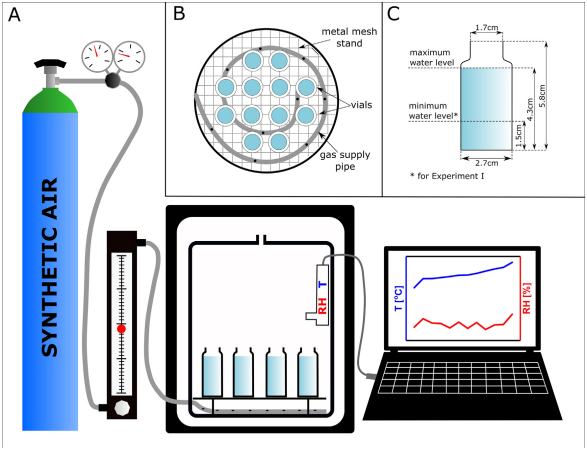

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Pierchala et al. '22 – triple isotope / kinetic fract. PySDM setup[a]

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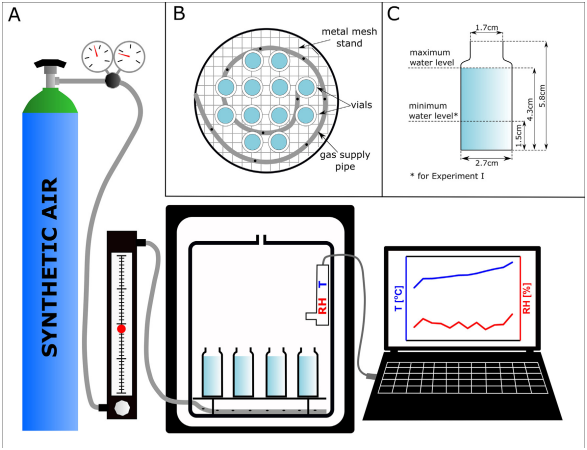

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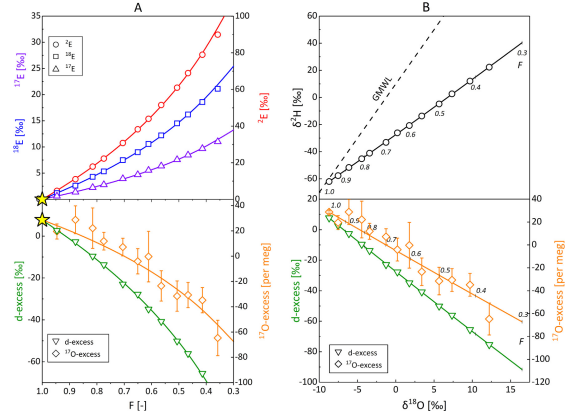

$$E = \frac{[\text{heavy iso.}]}{[\text{light iso.}]} \Big/ \frac{[\text{heavy iso.}]}{[\text{light iso.}]}\Big|_{t=0} - 1 \qquad \delta = \frac{[\text{heavy iso.}]}{[\text{light iso.}]} \Big/ \frac{[\text{heavy iso.}]}{[\text{light iso.}]}\Big|_{\text{VSMOW}} - 1$$

F: fraction of water remaining

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

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

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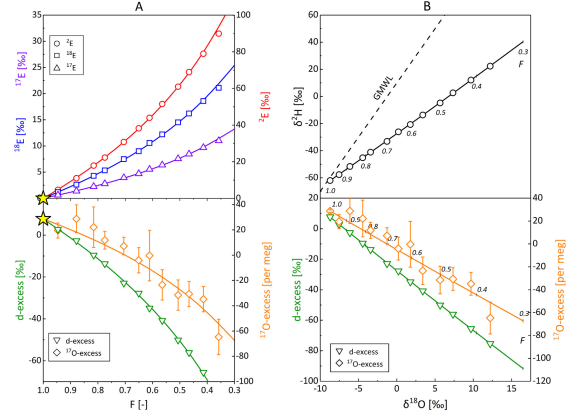
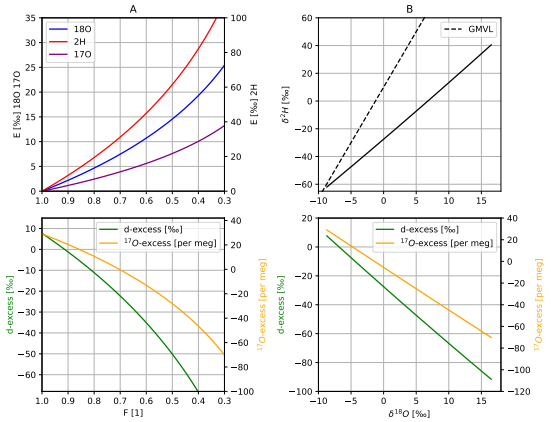


PySDM: theoretical curves



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

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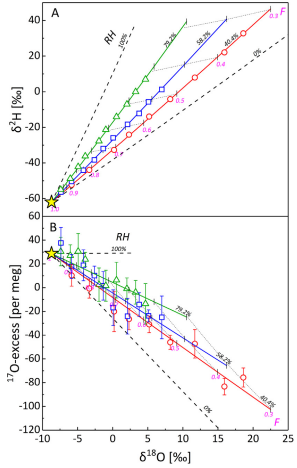
Fig. 4 (paper): RH varied



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

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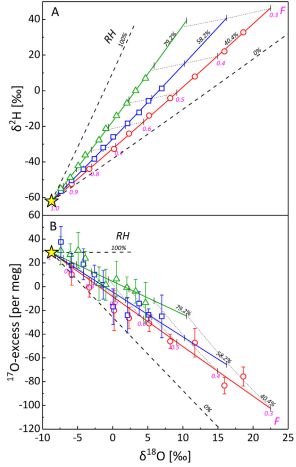
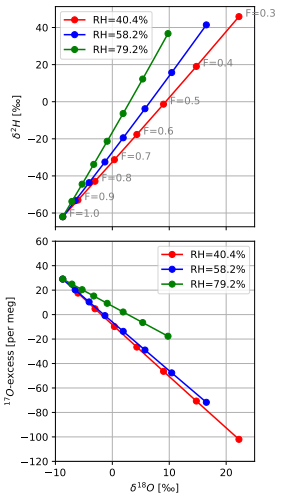


PySDM: model curves



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

pypi.org/p/PySDM-examples

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1D single-column kinematic env. (advection: PyMPDATA)								
Shipway & Hill 2012	×	×			×			#KiD
deJong et al. 2023 (figures 6-8)	×	×		×	×			#KiD
...								
2D prescribed-flow environment (advection: PyMPDATA)								
Arabas et al. 2015	×	×			×			#GUI
Arabas et al. 2023 (figure 11)	×	×			×		×	#Paraview

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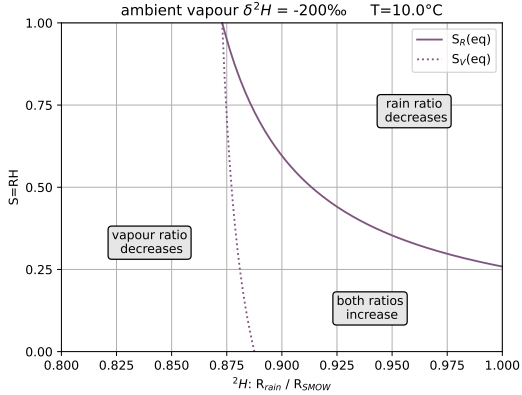
$$S_R \rightsquigarrow \frac{d\delta_{\text{rain}}}{dt} = 0$$
$$S_V \rightsquigarrow \frac{d\delta_{\text{vap}}}{dt} = 0$$



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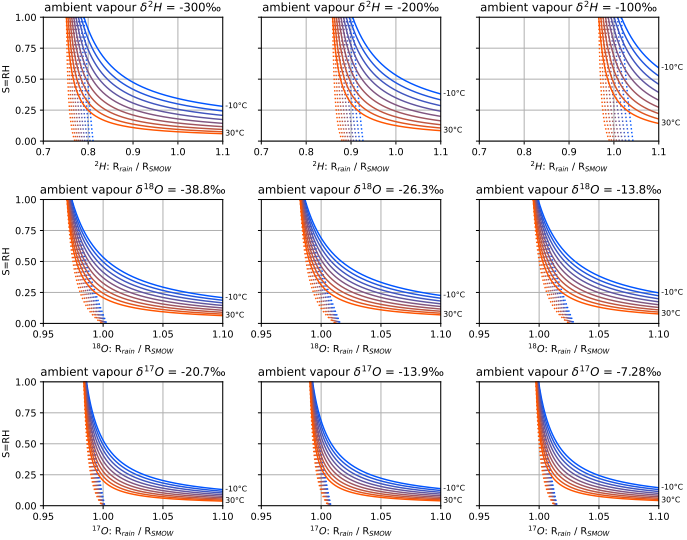

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motivation slide!

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 facetted 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 ±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

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merci de votre attention