Immersion freezing in particle-based cloud μ-physics models

S. Arabas[1] (ex-2), J.H. Curtis[2], I. Silber[3], A. Fridlind[4], D.A. Knopf[5], M. West[2] & N. Riemer[2]

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Immersion Freezing in Particle-Based Aerosol-Cloud Microphysics: A Probabilistic Perspective on Singular and Time-Dependent Models

Sylwester Arabas[1], Jeffrey H. Curtis[2], Israel Silber[3,4], Ann M. Fridlind[5], Daniel A. Knopf[6], Matthew West[7], and Nicole Riemer[2]

10.1029/2024MS004770

Aerosol-cloud interactions: a conceptual picture

Aerosol-cloud interactions: a conceptual picture

background image: vitsly.ru / Hokusai

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two-way interactions:
- aerosol characteristics influence cloud microstructure
- cloud processes influence aerosol size and composition

background image: `vitsly.ru` / Hokusai

Aerosol-cloud interactions: μ-physics models

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COMMISSIONED MANUSCRIPT
10.1029/2019MS001689

Key Points:
- Microphysics is an important component of weather and climate models, but its representation in current models is highly uncertain

Confronting the Challenge of Modeling Cloud and Precipitation Microphysics

Hugh Morrison[1], Marcus van Lier-Walqui[2], Ann M. Fridlind[3], Wojciech W. Grabowski[1], Jerry Y. Harrington[4], Corinna Hoose[5], Alexei Korolev[6], Matthew R. Kumjian[4], Jason A. Milbrandt[7], Hanna Pawlowska[8], Derek J. Posselt[9], Olivier P. Prat[10], Karly J. Reimel[4], Shin-Ichiro Shima[11], Bastiaan van Diedenhoven[2], and Lulin Xue[1]

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Particle-based μ-physics + prescribed-flow hello world

Lagrangian component

Eulerian component

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Shima et al. '20 particle-based mixed-phase μ-physics

Shima, Sato, Hashimoto & Misumi 2020 (GMD):

Predicting the morphology of ice particles in deep convection using the super-droplet method

Figure 1. Typical realization of CTRL cloud spatial structures at $t = 2040$, 2460, 3000, 4200, and 5400 s. The mixing ratio of cloud water, rainwater, cloud ice, graupel, and snow aggregates are plotted in fading white, yellow, blue, red, and green, respectively. The symbols indicate examples of unrealistic predicted ice particles (Sects. 7.3 and 9.1). See also Movie 1 in the video supplement.

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  — homogeneous and immersion freezing (singular)
  — melting
  — condensation and evaporation (incl. CCN [de]activation)
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Immersion freezing and other ice crystal formation pathways in clouds

Kanji et al. 2017, graphics F. Mahrt, https://doi.org/10.1175/AMSMONOGRAPHS-D-16-0006.1

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Immersion freezing: bacteria and the Olympics

Journal of Geophysical Research: Atmospheres

RESEARCH ARTICLE
10.1002/2016JD025251

Key Points:
- Very ice active Snomax protein aggregates are fragile and their ice nucleation ability decreases over months of freezer storage
- Partitioning of ice active protein aggregates into the immersion oil reduces the droplet's measured freezing temperature
- Caution is warranted in the use of

The unstable ice nucleation properties of Snomax® bacterial particles

Michael Polen[1], Emily Lawlis[1], and Ryan C. Sullivan[1]

[1]Center for Atmospheric Particle Studies, Carnegie Mellon University, Pittsburgh, Pennsylvania, USA

Abstract Snomax® is often used as a surrogate for biological ice nucleating particles (INPs) and has recently been proposed as an INP standard for evaluating ice nucleation methods. We have found the immersion freezing properties of Snomax particles to be substantially unstable, observing a loss of ice nucleation ability

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https://www.reuters.com/markets/commodities/making-snow-stick-wind-challenges-winter-games-slope-makers-2021-11-29/

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Vonnegut 1948 (J. Colloid Sci.)

Fraction of water drops remaining unfrozen as a function of time.

Szakáll et al. 2021, ACP 21: isothermal experiments

Marshall et al. 1961, Nubila 4(1)

Heterogeneous Nucleations is a Stochastic Process

by

J. S. MARSHALL

McGill University, Montreal, Canad.

Presented at the International Congress on the Physics of Clouds (Hailstorms) at Verona 9-13 August 1960.

http://cma.entecra.it/Astro2_sito/doc/Nubila_1_1961.pdf

Poissonian model of freezing & Ice Nucleation Active Sites (INAS)

theory (in modern notation)
(Bigg '53, Langham & Mason '58, Carte '59, Marshall '61)

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Poisson counting process with rate r:

$$P^*(\text{k events in time t}) = \frac{(rt)^k \exp(-rt)}{k!}$$

$$P(\text{one or more events in time t}) = 1 - P^*(k = 0, t)$$

$$\ln(1 - P) = -rt$$

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introducing $J_{\text{het}}(T)$, $T(t)$ and INP surface A:

$$\ln\left(1 - P(A, t)\right) = -A \underbrace{\int_0^t J_{\text{het}}(T(t'))\, dt'}_{I(T)}$$

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experimental $n_s(T)$ fits: e.g., Niemand et al. 2012

Particle-based freezing: singular (Shima et al.)

singular: INAS T_{fz} **as attribute**; initialisation by random sampling from $P(T_{\mathrm{fz}}, A)$ with lognormal A (A is not an attribute, initialisation only); freezing if $T(t) < T_{fz}(t = 0)$

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particle attribute sampling

particle attribute sampling
particle dynamics
random sampling of immersed surface for each particle
immersed surf. [μm²]
3.0
2.5
2.0
1.5
1.0
random sampling of freezing temperatures
(conditional distribution for a given surface)
attr: freezing temp. [K]
245
240
235
liquid
singular
frozen
(finite state machine)
deterministic transition
if T falls below Tf

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245
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liquid
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deterministic transition
if T falls below Tf
frozen fraction [1]
0.50
0.25
0.00
0
5
time [min]
temperature
singular
time-dep.

particle attribute sampling
particle dynamics
random sampling of immersed surface for each particle
immersed surf. [μm²]
3.0
2.5
2.0
1.5
1.0
random sampling of freezing temperatures
(conditional distribution for a given surface)
attr: freezing temp. [K]
245
240
235
(discrete time Markov chain)
$P_i = J_S(T) \cdot S_i \cdot \Delta t$
probability of transition
in each timestep
time-dependent
singular
liquid
frozen
(finite state machine)
deterministic transition
if T falls below Tf
frozen fraction [1]
0.50
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- Monte-Carlo: singular/INAS
- Monte-Carlo: time-dependent/ABIFM
- singular CDF for 0.1x median surface
- singular CDF for 1x median surface
- singular CDF for 10x median surface

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AIDA @ KIT

(https://www.imk-aaf.kit.edu/73.php, photo: KIT/Ottmar Möhler)

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singular (INAS)

time-dependent (J_{het})

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16+16 super-particles/cell for INP-rich + INP-free particles

$N_{\mathrm{aer}} = 300/cc$ (two-mode lognormal) $N_{\mathrm{INP}} = 150/L$ (lognormal, $D_g = 0.74$ μm, $\sigma_g = 2.55$)

spin-up = freezing off; subsequently frozen particles act as tracers

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- singular vs. time-dependent markedly different (consistent with box model for $c \ll 1K/min$)
- CPU time trade off: time dependent ca. 3-4 times costlier

100% python™ open-source code:

/ OPENATMOS / PySDM

The impact of aerosol mixing state on immersion freezing: Insights from classical nucleation theory and particle-resolved simulations

Wenhan Tang , Sylwester Arabas , Jeffrey H. Curtis , Daniel A. Knopf , Matthew West , and Nicole Riemer

Abstract. Immersion freezing, initiated by ice-nucleating particles (INPs) in supercooled aqueous droplets, plays an important role in the formation of ice crystals within clouds. The efficiency of immersion freezing depends strongly on INP composition and, crucially, on the mixing state—how chemical species are distributed across the particle population. Here, we quantify the impact of aerosol mixing state on immersion freezing using a combined theoretical and particle-resolved modeling approach.

(a): isothermal freezing conditions with −20 °C
(b): constant cooling rate from −10 °C to −30 °C within 10 minutes

Thank you for your attention!

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Immersion Freezing in Particle-Based Aerosol-Cloud Microphysics: A Probabilistic Perspective on Singular and Time-Dependent Models

Sylwester Arabas[1], Jeffrey H. Curtis[2], Israel Silber[3,4], Ann M. Fridlind[5], Daniel A. Knopf[6], Matthew West[7], and Nicole Riemer[2]

10.1029/2024MS004770

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