Ice Nucleation and Cloud Seeding: A Research Paper Built on Computer Experiments

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Abstract

This paper reports how far a researcher without a laboratory can get on the ice-nucleation question using computers alone, and where that approach stops. **No part of it is laboratory evidence; every number is a simulation or a sensitivity calculation.**

Question: Why do dust and biological particles start freezing at such warm temperatures, and how does this affect climate models, cloud seeding and agriculture? We designed a pilot droplet-freezing experiment (2 runs × 30 droplets) for a home freezer and simulated what that pilot could and could not distinguish.

Key findings: - **The pilot appears adequately powered for K-feldspar.** At 0.1% K-feldspar the probability of detecting a difference is 92–100% (assuming log10); for quartz at 0.1% it is only 10–40%. The false-positive rate on the same data is below 1%. - **Cooling rate is the largest hidden source of error.** Doubling the cooling rate can shift the freezing temperature by up to about 1 °C; small rate differences between surfaces produce false differences in fine comparisons. - **Composition matters as much as quantity.** A 10× increase in dust concentration warms the cloud-relevant INP threshold temperature by about 2.5–2.8 °C; a 10× increase in the K-feldspar fraction warms it by about 2.8 °C. - **In molecular dynamics (mW water, 1000 molecules), no confirmed crystallization was observed** within 29.5 ns at 185 K or 19 ns at 195 K.

What was not found: there is no real freezing data. The logarithm base of the Harrison et al. (2019) surface-density polynomials could not be verified from the source; log10 was assumed, and the results are sensitive to that assumption.

1. Introduction

Pure water can stay liquid far below 0 °C. Most cloud droplets are therefore still liquid at sub-zero temperatures; homogeneous freezing starts only below about −38 °C. For ice to form at warmer temperatures, an ice-nucleating particle (INP) is needed. The number and type of these particles set the liquid-to-ice ratio in mixed-phase clouds, and with it the sunlight a cloud reflects and how long it lives. This link sits at the center of three debates: cloud feedback in climate models, whether cloud seeding works, and frost damage to crops.

Central claim. The first ice crystal rarely forms on its own; a surface or particle almost always takes part. A particle’s effectiveness depends less on its mass than on nanoscale active sites on its surface (cracks, steps, hydrophobic patches, protein clusters).

Testable hypotheses (all falsifiable): - **H1:** At equal mass concentration, K-feldspar suspension droplets freeze at a higher median temperature than quartz and kaolin. - **H2:** Boiling a garden-soil extract lowers its freezing temperature (an indicator of a biological contribution); pure K-feldspar is not noticeably affected by boiling. - **H3:** The same pure-water droplet freezes at a warmer temperature on a scratched surface than on a smooth one (the weakest hypothesis).

Scope. Without laboratory access, H1–H3 were not tested. Instead we (i) surveyed the literature, (ii) designed a pilot for a home experiment and simulated its power, (iii) examined two major error sources (cooling rate, dust composition) with sensitivity calculations, and (iv) assessed the feasibility of molecular dynamics with the mW water model.

2. Literature

Only the abstracts of the sources were read; no number should be treated as firm without reading the full text.

2.1 Mineral dusts and biological nucleators

Topic	Finding	Source
Mineral dusts	K-feldspar is by far the most active mineral in immersion freezing; quartz is much weaker but so abundant in dust that it can contribute meaningfully to global INP	ACP 23, 1785 (2023)
Quartz	Across 10 α-quartz samples, freezing temperature at constant active-site density varies by about 12 °C; quartz is typically about 7 °C less active than K-feldspar	Harrison et al., ACP 19, 11343 (2019)
Variation within feldspar	Alkali/K-rich feldspar samples are the most active; even among K-rich samples there is scatter	Harrison et al., ACP 16, 10927 (2016)
Size	Microcline shows immersion freezing even at 50 nm	ACP 19, 10901 (2019)
Solutes	Solutes can change feldspar activity	ACP 18, 7057 (2018)
Biological	INA bacteria (e.g. *P. syringae*) are among the most active known nucleators; they can freeze water at about −2 °C	PMC7895962; Bieber & Borduas-Dedekind (2024)
Heat test	K-feldspar is not noticeably affected by wet heating, but quartz and plagioclase lose activity; equating loss after heating with a biological origin can be misleading	Daily et al., AMT 15, 2635 (2022)

Open scientific questions: why K-feldspar is so active (Kiselev et al. 2017 proposed epitaxy and surface defects; later MD studies did not find this on the (100) surface; a preprint proposes the (110) surface, not peer-reviewed) and how INA proteins nucleate ice are both still debated.

2.2 Climate link

- Frostenberg et al. (2026) report that the dominant microphysical processes governing mixed-phase clouds differ widely across three climate models.
- Murray, Carslaw & Field (ACP 2021): in a warming world, clouds shift toward more liquid water, producing a negative “cloud-phase” feedback whose size depends on the ice-nucleating aerosol fraction.
- McGraw et al. (GRL 2023, CESM2): nucleation affects cloud feedbacks, but once cloud phase is tuned to satellite observations, the total cloud feedback is not very sensitive to the choice of nucleation scheme.
- Kok et al. (2023): models do not represent the historical increase in dust, which can bias climate-sensitivity estimates.

Implication: “INP knowledge determines climate sensitivity” is too strong. INPs are an important source of uncertainty in the cloud-phase feedback, but in some models the total cloud feedback is not very sensitive to them.

2.3 Cloud seeding and agriculture

- US GAO report (December 2024): estimated additional precipitation in the studies reviewed is 0–20%; efficacy data are missing or unreliable.
- Knowles & Skidmore (North Dakota): wheat and barley yields rose in seeded counties; **but this is an observational panel regression, not a randomized assignment**, so the evidence for causation is weak.
- Frost and agriculture: INA bacteria can trigger frost on leaves between −2 and −5 °C (UC ANR; Lindow et al.); this is the most solid agricultural link.

We **did not find** a reliable source on long-term regional side effects (such as downwind precipitation); that means “not found,” not “does not exist.”

3. Methods

3.1 Planned home experiment (not carried out)

A droplet-freezing assay in a home freezer: same shelf, same run, 30 droplets on a separate surface for each condition, one sensor per surface, phone video. Pre-specified metric: median freezing temperature per condition (T50). Decision rule: the difference must be at least twice the between-run standard deviation of the blank-droplet T50 (floor 1.0 °C); otherwise “could not be distinguished.” A home freezer reaches about −18 °C; hitting that floor is itself a result, not an error.

3.2 Computer experiments

#	Experiment	What was done
1	Pilot design	Singular model (Poisson): expected active sites = ns(T)·A; Harrison et al. (2019) polynomials (quartz −10.5 to −37.5 °C; K-feldspar −3.5 to −37.5 °C; log(ns) SD 0.8); 20 µL droplets, 1 m²/g, background freezing ~N(−12 or

#	Experiment	What was done
		−15, 2 °C), run-to-run drift SD 0.6 °C, freezer floor −18 °C; 600 repetitions
3	Cooling rate	Time-dependent “hard” model, upper bound: about 3.3 °C shift per 10× change in rate
4 / 4b	Molecular dynamics	LAMMPS, mW water (Stillinger–Weber; Molinero & Moore 2009), 1000 molecules, NPT, rapid quench
5	Dust sensitivity	Temperature at which INP concentration reaches 1/L, varying dust amount and K-feldspar fraction

(Experiment 2: synthetic data generated only to test the analysis script; no scientific finding.)

3.3 Validation

- **mW parameters:** compared with Molinero & Moore 2009 (arXiv 0809.2811) and the NIST record; density at 300 K is 1.000 g/cm³ (reference ~0.997).
- **Harrison polynomials:** coefficients match the printed paper; **the logarithm base could not be verified because it is not stated**, so log10 was assumed and a sensitivity test with ln was run.
- **Analysis script:** the cooling-rate covariate was validated with tests written first; 3 tests pass.

4. Results

All results are simulations; there is no laboratory data.

4.1 Pilot power (2 runs × 30 droplets)

“P” is the probability that the T50 difference from the blank droplet is detected under the decision rule (600 repetitions). Median ΔT50 is given for the log10 assumption only.

Background (°C)	Mineral	Concentration (%)	Median ΔT50 (°C, log10)	P (log10)	P (ln)
−12	K-feldspar	0.01	1.48	0.53	0.18
−12	K-feldspar	0.1	4.13	0.92	0.76
−12	K-feldspar	1	6.92	1.00	0.98
−12	Quartz	0.01	0.06	0.01	0.02
−12	Quartz	0.1	0.36	0.10	0.18
−12	Quartz	1	1.15	0.41	0.51
−15	K-feldspar	0.01	3.70	0.90	0.40

Background (°C)	Mineral	Concentration (%)	Median ΔT50 (°C, log10)	P (log10)	P (ln)
−15	K-feldspar	0.1	6.89	1.00	0.88
−15	K-feldspar	1	10.09	1.00	1.00
−15	Quartz	0.01	0.29	0.07	0.06
−15	Quartz	0.1	1.08	0.40	0.42
−15	Quartz	1	3.52	0.85	0.89

- For 1% K-feldspar the design catches the difference under both logarithm bases; in the 0.01–0.1% range the power depends strongly on the base.
- The blank droplet's own freezing temperature is the biggest unknown.
- With no mineral added (null case), the false-positive rate is below 1%.

4.2 Cooling rate

- Doubling the cooling rate shifts T50 by about 1 °C (the **upper bound** of the time-dependent "hard" model).
- Even when the same sample is on two surfaces, the probability of a false difference rises from 0.7% to 15.8% as the rate difference between surfaces grows (surface-rate SD 0 → 0.3; K-feldspar 0.1%).
- The mineral-versus-blank difference stays robust; **fine comparisons (H2, H3) are fragile to rate differences between surfaces**: at a 1.6× rate difference the false difference is 6–8%.
- Conclusion: a sensor on every surface, log `cooling_rate_K_per_min`, apply a rate correction; for H2/H3 use a 1.5–2 °C threshold.

4.3 Dust sensitivity (INP = 1/L threshold, assuming log10)

- Each 10× increase in dust warms the threshold by about 2.5–2.8 °C (−26.3 → −23.5 → −20.9 °C).
- K-feldspar fraction 0.5% → 5% (10×) warms it by about 2.8 °C.
- Quartz-only dust: −31.8 °C; mix with 5% K-feldspar: −23.5 °C. **Composition matters as much as quantity.**
- Under ln the threshold is not reached down to −37.5 °C; these numbers are conditional on log10.

4.4 Molecular dynamics (mW water)

T (K)	Duration	Result
190 and 200	6 ns	No crystallization observed
185	29.5 ns	No flag; PE/molecule ≈ −11.13 → −11.21 kcal/mol, density steady ≈ 0.97 g/cm³
195	19.0 ns	Flag raised, but not trusted: PE drifted slowly (−11.03 → −11.46), density unchanged

We could not verify the 195 K flag structurally (no coordinates saved); it is also consistent with slow structural relaxation. **Crystallization was not demonstrated.** One run of 1000 molecules says nothing about the nucleation rate.

5. Discussion

A home experiment can say nothing directly about global warming; it is a test of *mechanism*.

Link	Claim	Evidence level
1. Mechanism	Some particles (K-feldspar, INA bacterial proteins) start freezing at very warm temperatures	Strong (laboratory, many studies)
2. Cloud phase	INP amount sets the liquid/ice ratio of mixed-phase clouds	Strong, but inconsistent across models
3. Cloud-phase feedback	Warming shifts clouds from ice to liquid and albedo rises (negative feedback); size depends on INP	Contested
4. Global warming	The size of this feedback affects climate sensitivity	Contested, not decisive alone
5. Agriculture (frost)	INA bacteria raise the temperature of leaf frost damage	Strong
6. Agriculture (seeding)	Seeding increases yield	Weak to moderate (observational, limited)

Where do our findings sit? - *Link 1:* composition (K-feldspar fraction) matters as much as quantity, so “dust” in a model is not one number; conditional on the log base. - *Links 2–4:* our simulations do not touch these; we carry only the literature and the “source of uncertainty” framing. - *Link 5:* the boiling test in H2 is a cheap kitchen probe of the biological contribution; but loss after heating alone does not mean “biological.” - *Link 6:* no new evidence on seeding efficacy; we note the weakness of the existing evidence.

Original open question (agriculture → climate): Is the ice-nucleating activity of agricultural soil extracts sensitive to heating? Agricultural dust can contain organic matter and may behave differently from desert dust (Liu et al., AMS 2024 presentation; not peer-reviewed). This ties directly to H2 and is a cheap start for someone with laboratory access.

6. Limitations and honest notes

- **No real data.** Every number is a simulation or sensitivity calculation; H1–H3 were not tested.
- **Logarithm base not verified.** For K-feldspar at −15 °C, log10 gives ns ≈ 350 cm^{-2} and ln ≈ 13 cm^{-2}; the order of magnitude recalled from the literature (not confirmed) makes log10 more likely but does not prove it.
- **Assumptions:** 20 µL droplet, 1 m^2/g, background-freezing distribution and run-to-run drift; update with real blank-droplet data.
- **The cooling-rate model is an upper bound.**

- **MD:** a single run, 1000 molecules, an arbitrary crystallization threshold (PE drop); no structural validation (q6, coordinate dumps).
- **Reading depth:** abstracts only; preprints are not peer-reviewed.
- **Climate claim:** a home experiment does not represent atmospheric conditions; it is a hypothesis test, not a calibrated INP measurement.

7. Conclusion and next steps

The most important thing that could be done without a laboratory was to know in advance what an experiment can distinguish. The pilot can probably detect a K-feldspar effect (assuming log10) but struggles with quartz, and the cooling rate and blank-droplet baseline shape the result as much as the setup. The dust experiment suggested that cloud ice formation may be more sensitive to dust composition than amount. The MD side produced no nucleation statistics on this machine.

Next steps: 1. Pilot: one surface (cling film), microcline and blank water, 30 droplets each; a sensor on every surface and a `cooling_rate_K_per_min` log; analyze with `analyze_freezing.py`. 2. Pin down the log base by comparing the polynomial with Fig. 7 of Harrison et al. (2019). 3. MD: a longer multi-replica run detecting crystallization with q6 and coordinate dumps.

References

Harrison et al. 2019 (ACP 19, 11343) https://acp.copernicus.org/articles/19/11343/2019/ · Molinero & Moore 2009 https://arxiv.org/abs/0809.2811 · Harrison et al. 2016 https://acp.copernicus.org/articles/16/10927/2016/acp-16-10927-2016.xml · ACP 23, 1785 https://acp.copernicus.org/articles/23/1785/2023/ · ACP 19, 10901 https://acp.copernicus.org/articles/19/10901/2019/acp-19-10901-2019.pdf · ACP 18, 7057 https://acp.copernicus.org/articles/18/7057/2018/ · Kiselev et al. 2017 https://heibib.ub.uni-heidelberg.de/search/Record/1560698667 · K-feldspar (110) preprint https://arxiv.org/abs/2511.13402 · INA bacteria https://www.ncbi.nlm.nih.gov/pmc/articles/PMC7895962/ and https://www.ncbi.nlm.nih.gov/pmc/articles/PMC11221516/ · Daily et al. 2022 https://amt.copernicus.org/articles/15/2635/2022/ · Frostenberg et al. 2026 https://research.chalmers.se/en/publication/551413 · Murray et al. 2021 https://acp.copernicus.org/articles/21/665/2021/ · McGraw et al. 2023 https://duo.uio.no/handle/10852/108293 · Kok et al. 2023 https://escholarship.org/uc/item/85q3v8qp · GAO-25-107328 https://gao.gov/products/gao-25-107328 · Knowles & Skidmore https://www.sciencegate.app/document/10.1175/wcas-d-21-0010.1 · UC ANR https://ucanr.edu/node/101740 · Liu et al. 2024 https://ams.confex.com/ams/104ANNUAL/webprogram/Paper436478.html

All code, logs and reports are in the local folder `D:\bktm\Buz çekirdeklenmesi ve bulut tohumlama`.