Kinetic Nucleation in Thermal Non-Equilibrium

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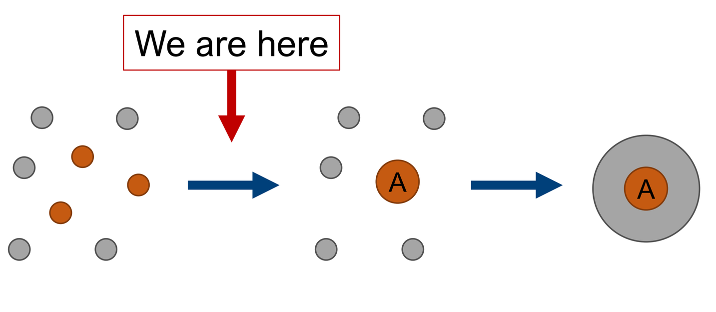
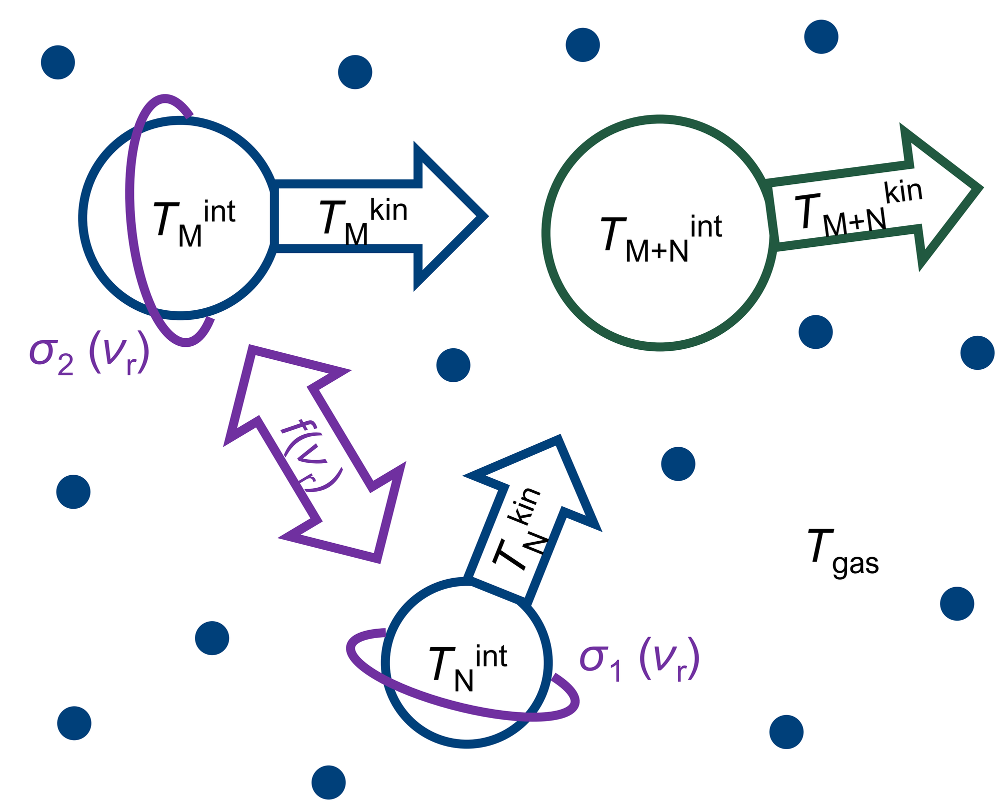
Take home Kinetic nucleation is affected by internal and kinetic temperatures of clusters and temperature differences between cluster sizes. Nonetheless, the assumption of thermal equilibrium is generally justified for exoplanet atmospheres.

Connection to Exoplanets

Clouds form when materials (●) condense onto aerosols (Ⓐ). In gaseous exoplanets, aerosols must form from the gas phase (●) via kinetic nucleation. With this work we look at the effect of thermal non-equilibrium.



Background



Growth reaction rate k^+:

- T^{int} internal temperature
- T^{kin} kinetic temperature
- T_{gas} gas temperature
- N, M, $N+M$ cluster sizes
- v_r relative velocity between colliding particles
- σ_j (v_r) reaction cross section
- f (v_r) velocity distribution

$$k_j^+ = \int_0^\infty \sigma_j(v_r)\, v_r\, f(v_r)\, dv_r$$

Where it gets complicated

Basis

$$k^- = k^+ \alpha \frac{p^\star}{kT_{gas}} ABC$$

Reverse reaction rate k^-:

- the principle of detailed balance
- chemical equilibrium as reference state [2]
- law of mass action including thermal non-equilibrium effects

Thermal equilibrium

$$A = \exp\left(\frac{G^\star_{(N+M)}(T^{kin}_{(N+M)}, p^\star)}{RT^{kin}_{(N+M)}} - \frac{G^\star_N(T^{kin}_N, p^\star)}{RT^{kin}_N} - \frac{G^\star_M(T^{kin}_M, p^\star)}{RT^{kin}_M} \right)$$

Kinetic-to-gas non-equilibrium

$$B = \exp\left(\frac{(T^{kin}_{(N+M)} - T_{gas})}{T^{kin}_{(N+M)}} - \frac{(T^{kin}_N - T_{gas})}{T^{kin}_N} - \frac{(T^{kin}_M - T_{gas})}{T^{kin}_M} \right)$$

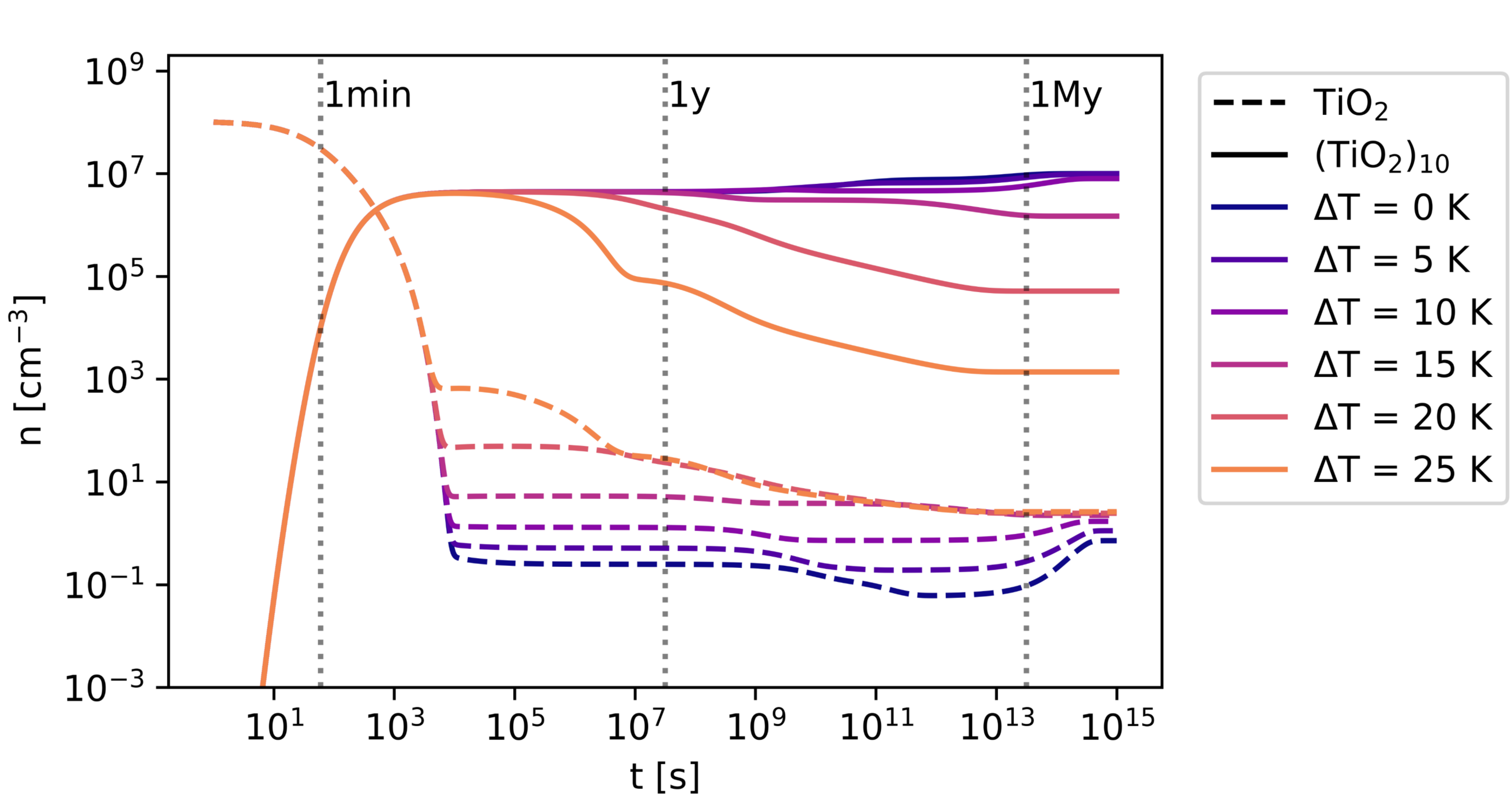
Internal-to-kinetic non-equilibrium

$$C = \exp\left(- \frac{\omega_{(N+M)}(T^{kin}_{(N+M)}, T^{int}_{(N+M)})}{kT^{kin}_{(N+M)}} + \frac{\omega_N(T^{kin}_N, T^{int}_N)}{kT^{kin}_N} + \frac{\omega_M(T^{kin}_M, T^{int}_M)}{kT^{kin}_M} \right)$$

Parameters used:

- standard pressure $p^\star = 10^5$ Pa
- cluster sizes N, M, $N+M$
- Gibbs free energy [4] $G_N^\star$ (T_N^{kin}, $p^\star$)
- Internal change in Gibbs free energy ω_N (T_N^{kin}, T_N^{int})
- Gibbs free energy gauge α

Results



Assumptions for this example:

- TiO_2 nucleation in a H_2 gas at T_{gas} = 1000 K
- Initial number density $n_{TiO_2} = 10^8$ cm^{-3}
- Internal-to-kinetic equilibrium $T_N = T_N^{kin} = T_N^{int}$
- Temperature offset $\Delta T = T_{(TiO_2)_{10}} - T_{TiO_2}$

Conclusions

- Thermal non-equilibrium can enhance or reduce $(TiO_2)_{10}$ formation.
- Kinetic nucleation in hot, low-density environments (like AGB stars [5]) can be affected by thermal non-equilibrium.
- Thermal equilibrium is a good assumption for exoplanet atmospheres.

Get in Touch!

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References

[1] Boulangier J. et al. 2019, MNRAS 489, 4890
[2] Patzer et al. 1998, A&A 337, 847P
[3] Burke & Hollenbach, 1983, ApJ 265, 223
[4] Lee et al. 2015, A&A 575, A11
[5] Fonfría J. P. et al. 2021, A&A 651, A8

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