Kinetic Nucleation in Thermal Non-Equilibrium

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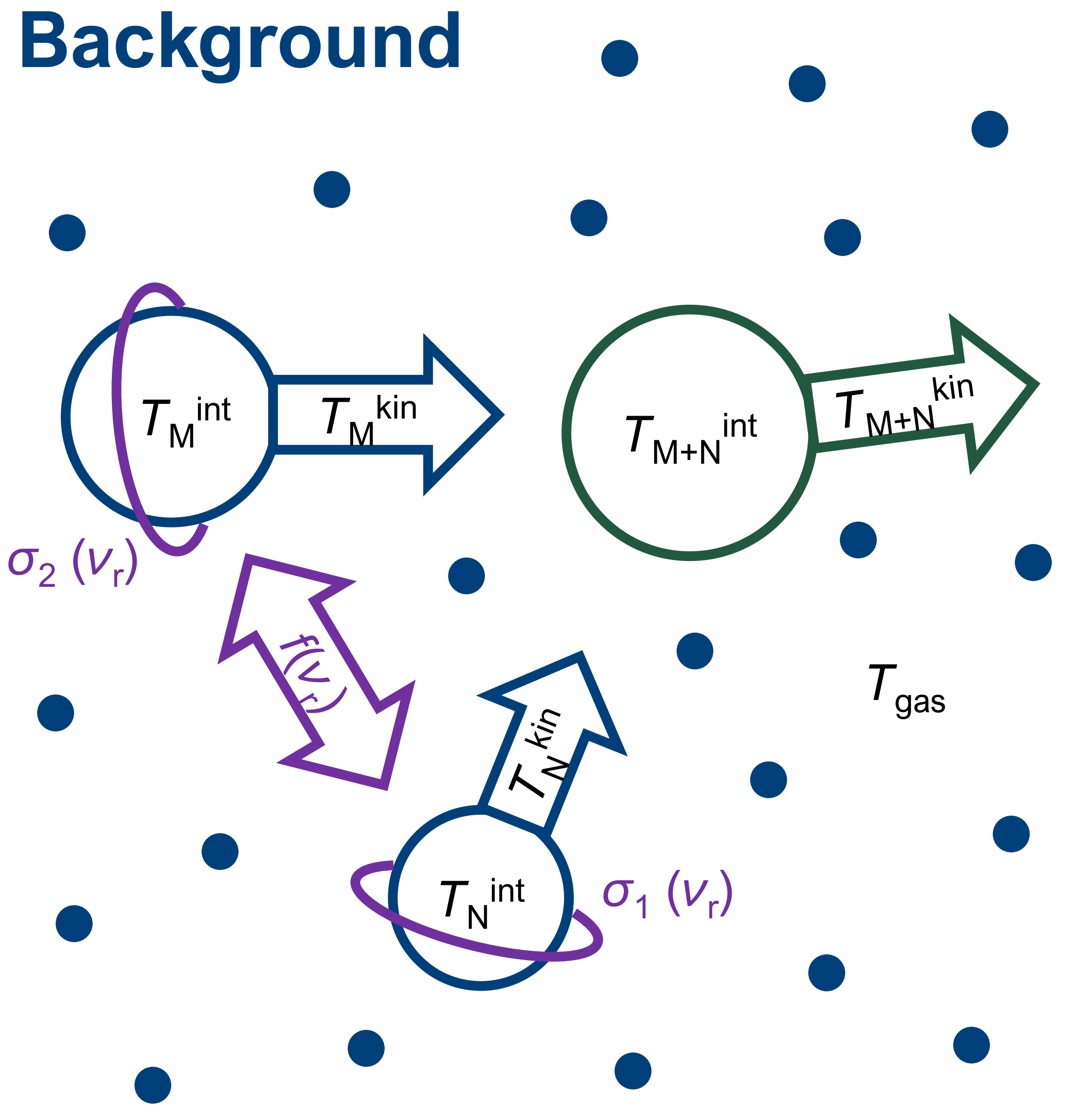
Take home Kinetic nucleation is affected by internal and kinetic temperatures of clusters and temperature differences between cluster sizes. Nonetheless, the assumption of thermal equilibrium is generally justified for exoplanets.

Background



Temperature

T^{int}, T^{kin}, T_{gas}	internal, kinetic & gas temperature
E^{tot}, E^{kin}, E^{int}	total, kinetic & internal energy
N, M, $N{+}M$	cluster sizes
D_N^{f}	internal degrees of freedom
k	Boltzmann constant

$$E_N^{\text{tot}} = E_N^{\text{kin}} + E_N^{\text{int}} = \frac{3}{2} k T_N^{\text{kin}} + \frac{D_N^f}{2} k T_N^{\text{int}}$$

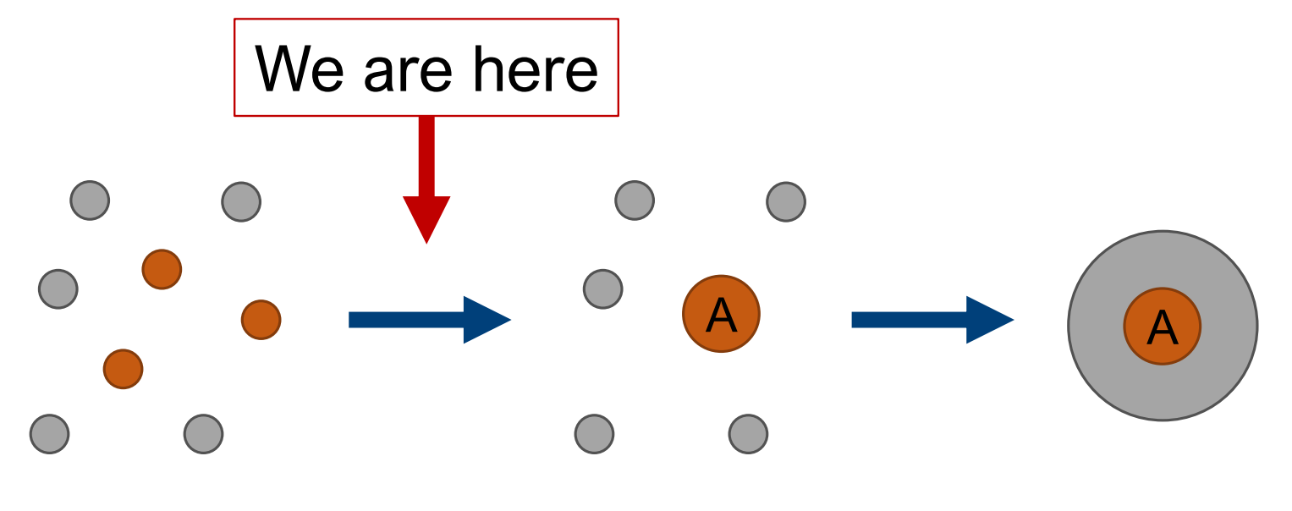
The forward (growth) reaction rate k^+:

v_r	relative velocity between colliding particles
$\sigma_j\,(v_r)$	reaction cross section
$f\,(v_r)$	relative velocity distribution

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

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.



Where it gets complicated

Basis

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

Thermal equilibrium

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

Kinetic-to-gas non-equilibrium

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

Internal-to-kinetic non-equilibrium

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

Parameters used:

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

The reverse reaction rate k^- is derived using:

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

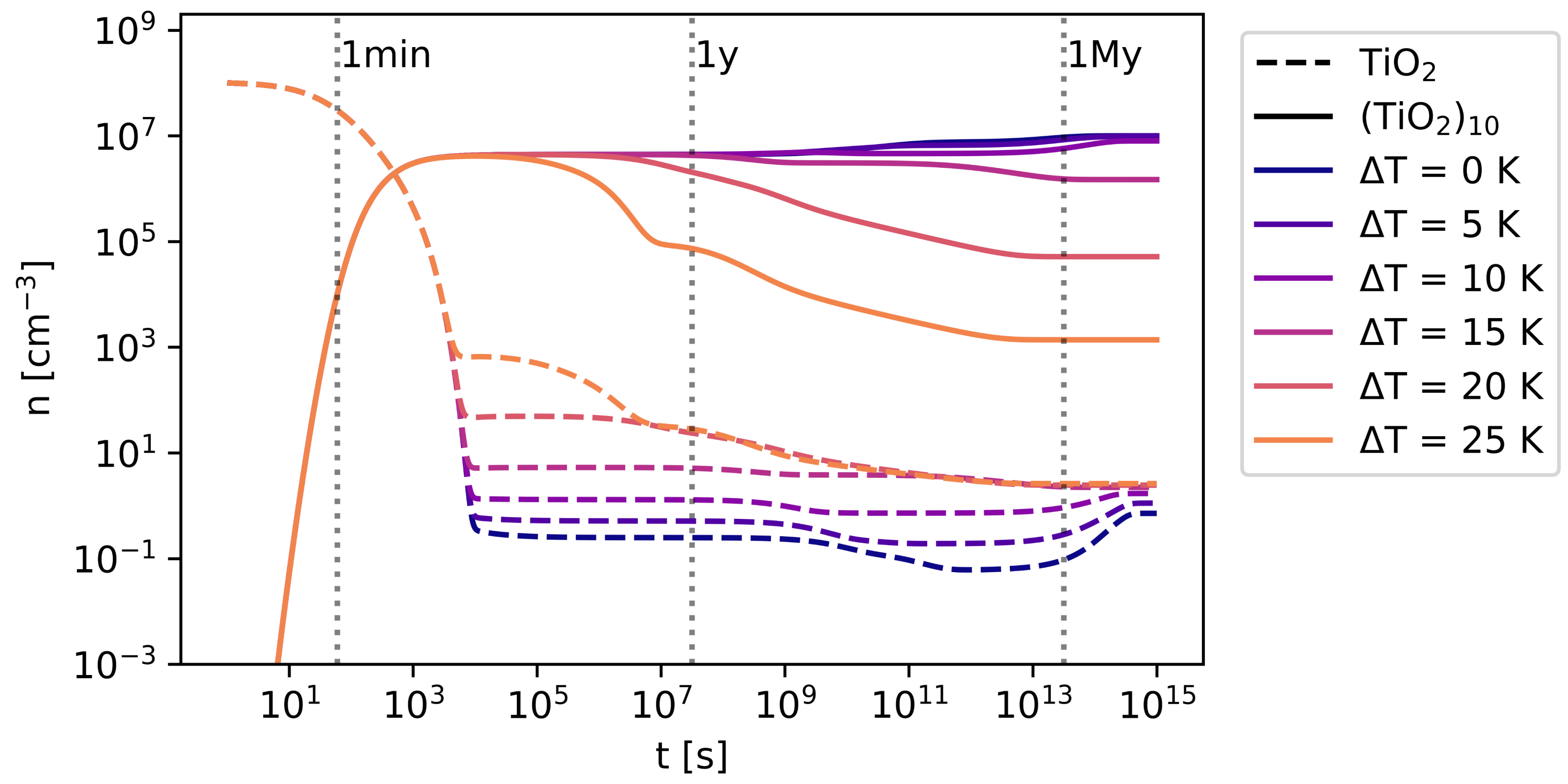
Results

Assumptions for this example:

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

Conclusions:

- Thermal non-equilibrium can enhance or reduce $(TiO_2)_{10}$ formation.
- Internal-to-kinetic thermal non-equilibrium affects the number density more than kinetic-to-gas thermal non-equilibrium.



Get in Touch!

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Acknowledgements

The authors want to thank Julian Lang for his help and contribution. S.K., L.D and C.H. acknowledge funding from the European Union H2020-MSCA-ITN-2019 under grant agreement no. 860470 (CHAMELEON). L.D and D.G. acknowledges support from the ERC consolidator grant 646758 AEROSOL.

References

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