Water Ice Sublimation and O-H Isotopic Fractionation in Terrestrial and Extraterrestrial Environments: New insights gained from numerical modelling and laboratory experiments

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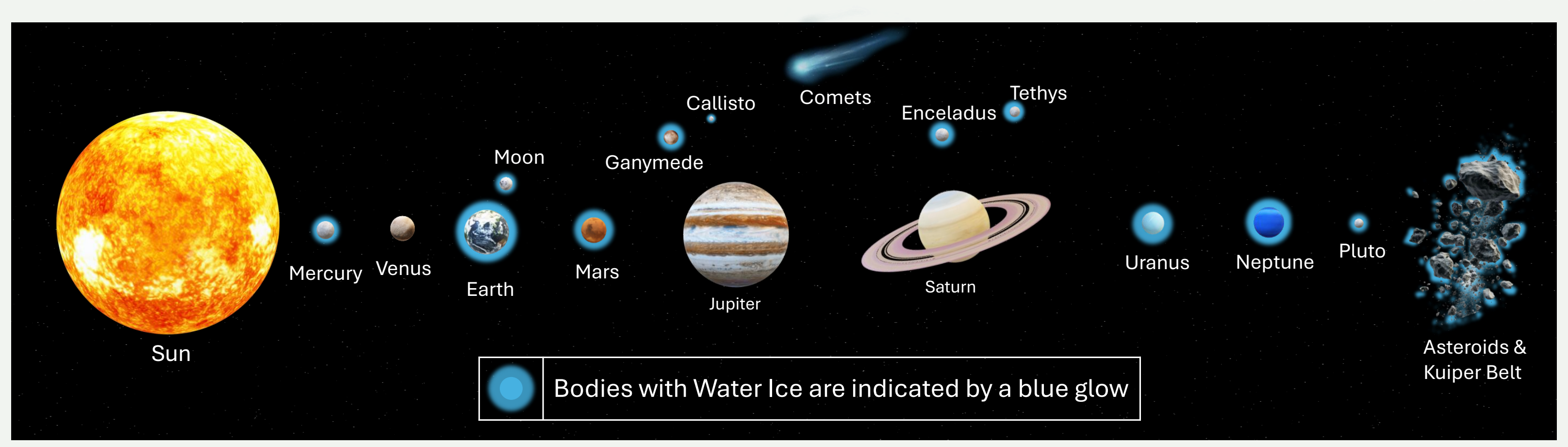
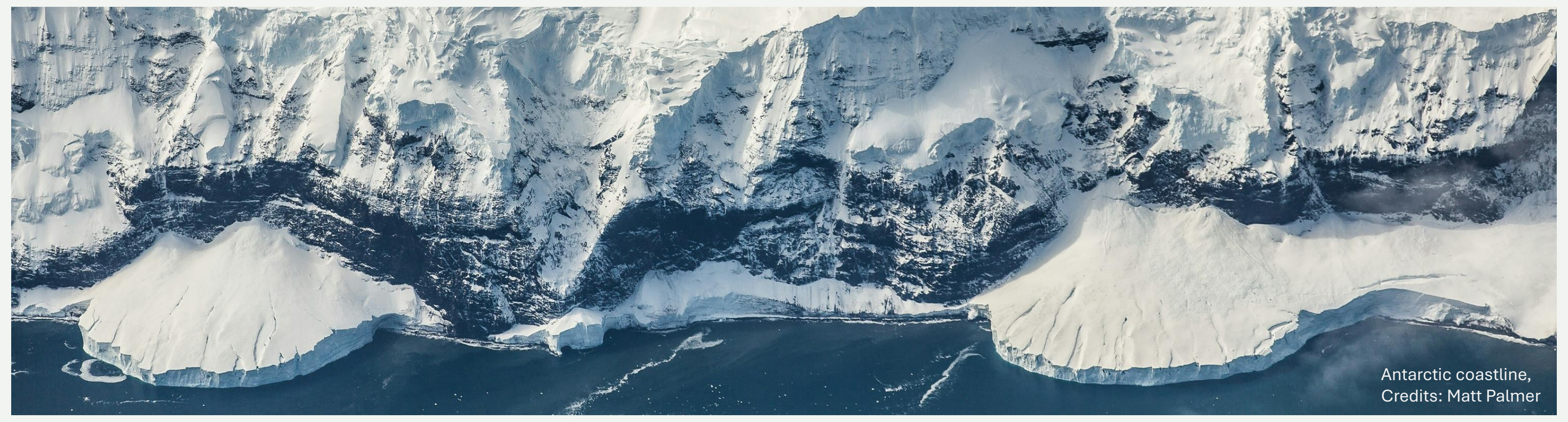
1. Introduction

- Tremendously large reservoirs of **extraterrestrial water ice** exist on previously supposed bone dry solar and extrasolar bodies serving as quintessential **resources** for space exploration.



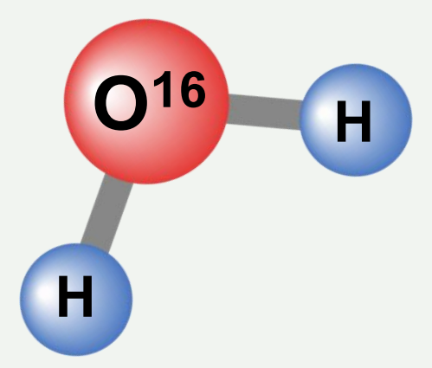
Bodies with Water Ice are indicated by a blue glow

- **Terrestrial water ice** (glaciers, permafrost, snow etc.) store valuable **climatological records** on timescales of a few days up to over hundreds of thousands of years.

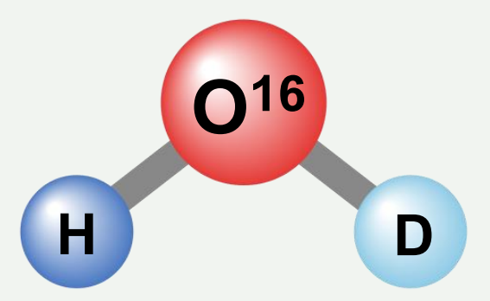


Antarctic coastline, Credits: Matt Palmer

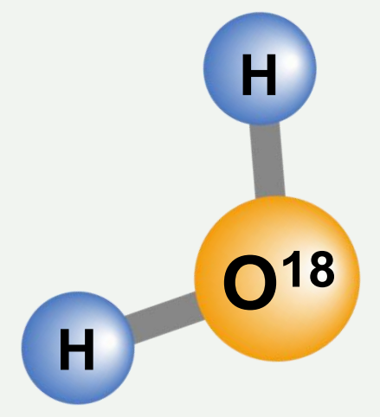
- **Stable isotopes** of oxygen and hydrogen (**O-H**) are powerful **tracers** of natural phenomena widely used across multiple disciplines in Earth and Planetary sciences.



$M_{H_2O_{16}}$ = 2.99 × 10^{-26} kg
Natural abundance = 99.7310 %



$M_{HDO_{16}}$ = 3.16 × 10^{-26} kg
Natural abundance = 0.0037 %



$M_{H_2O_{18}}$ = 3.32 × 10^{-26} kg
Natural abundance = 0.2000 %

2. Motivation

- **Few experimental studies** investigated **water ice sublimation** rates and **O-H isotopic fractionation** under extreme conditions like the **lunar environment**.
- **Many unknowns and uncertainties** in sublimation - fast diffusion - condensation of water ice and related O-H isotopic fractionation under extreme low temperatures and vacuum.
- Experimental and numerical modelling approaches will help **guide space technologies** for water ice extraction and **inform climate science** in past climate reconstructions.

3. Experiments

LUNAQUA is a laboratory scale prototype developed at LIST, capable of producing ultra high vacuum **(UHV~10^{-7} Pa)** and cryogenic temperatures **(~110 K)**, fig. **(a)**.

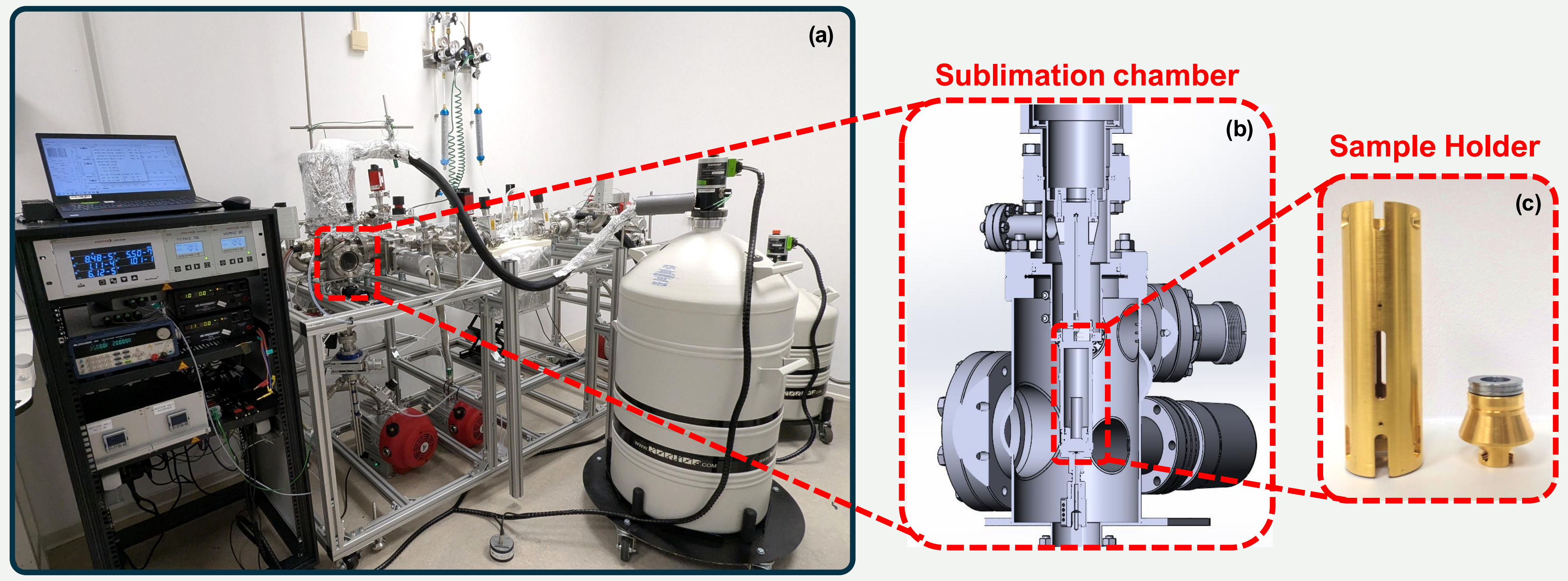
Step 1: Water ice samples of different isotopic compositions ($\delta^{18}O$ and $\delta^{2}H$) are introduced in the prototype's sublimation chamber [fig. **(b)**] within a sample holder [fig. **(c)**] and sublimated **(T_{sub} ~195 K)**.

Step 2: A cold trap on the other end at ~90K condenses the sublimated water vapor.

Step 3: Fully and sequentially condensed water is analysed for $\delta^{18}O$ and $\delta^{2}H$ values.

$$\delta^{A}X = \frac{R_{Sample}}{R_{Standard}} - 1\ (\times 10^{3}‰) \qquad R = \frac{Abundance\ of\ rare\ isotope}{Abundance\ of\ abundant\ isotope} \qquad \alpha_{sub} = \frac{R_{vapor}}{R_{ice}}$$

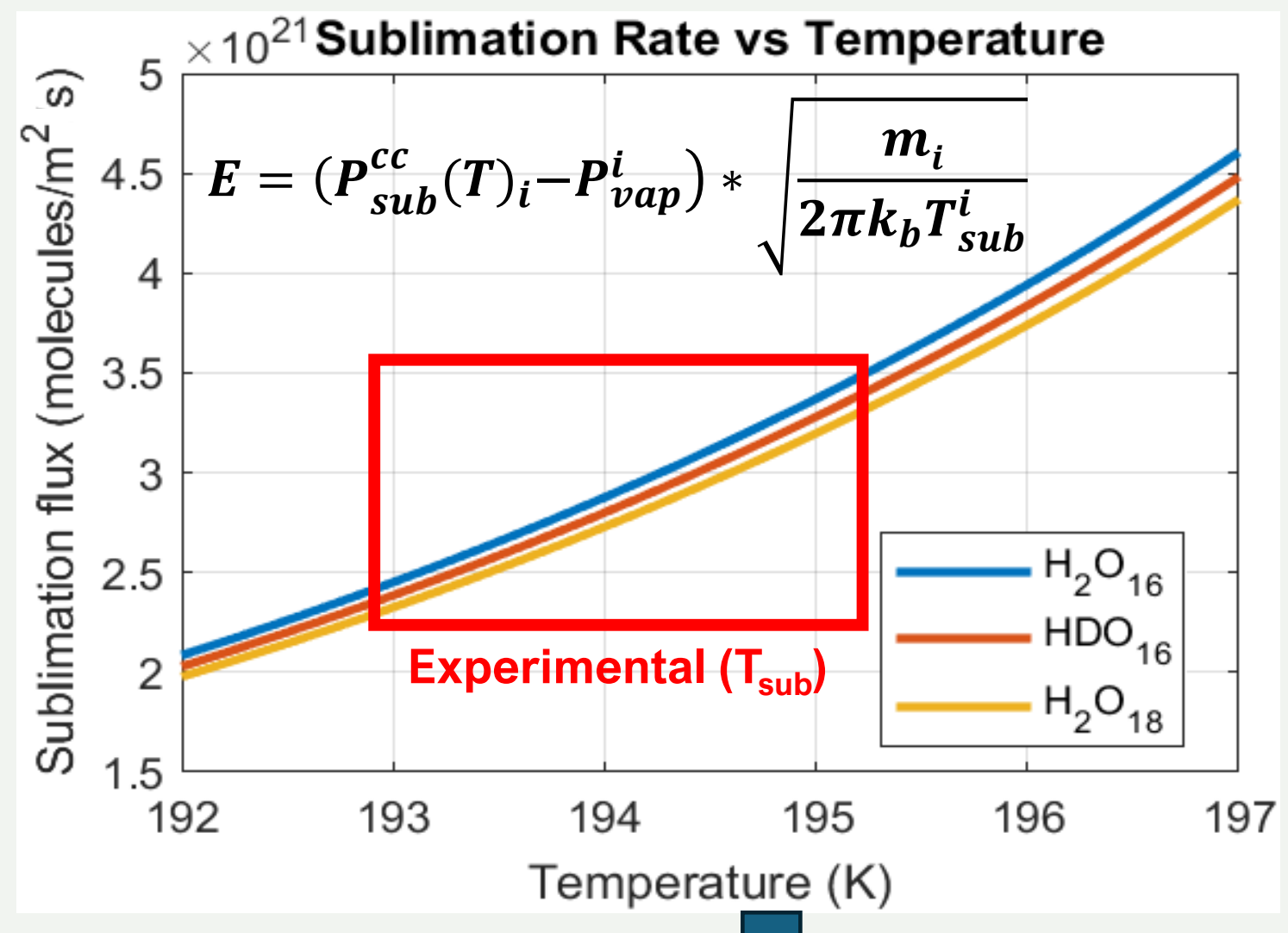
LUNAQUA Prototype



4. Numerical Modelling

Step 1: Sublimation Rate

(Hertz-Knudsen Equation)



$$E = \left(P^{cc}_{sub}(T)_i - P^{i}_{vap}\right) * \sqrt{\frac{m_i}{2\pi k_b T^{i}_{sub}}}$$

Step 2: Lagrangian Tracking:

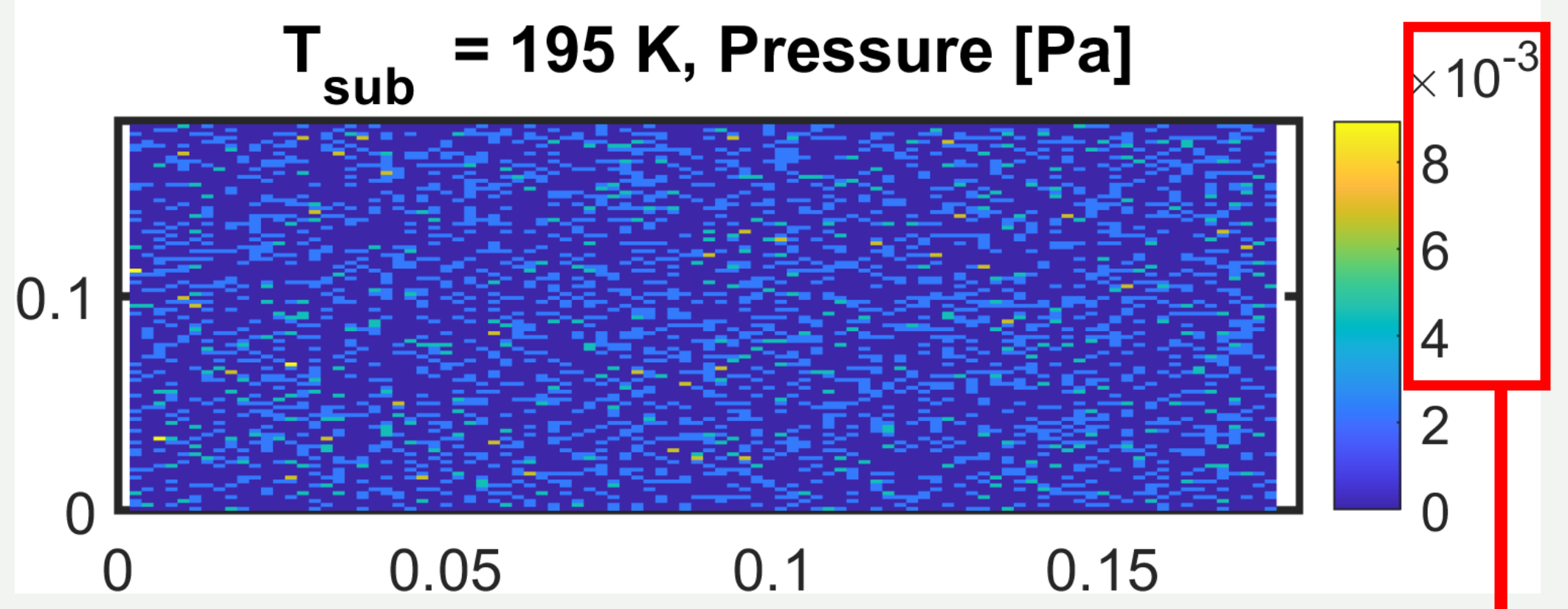
(Langevin's equation) **(Vacuum)**

$$x_{new} = x_{old} + v_{Boltz} * \Delta t + \cancel{v_{darcy} * \Delta t}$$

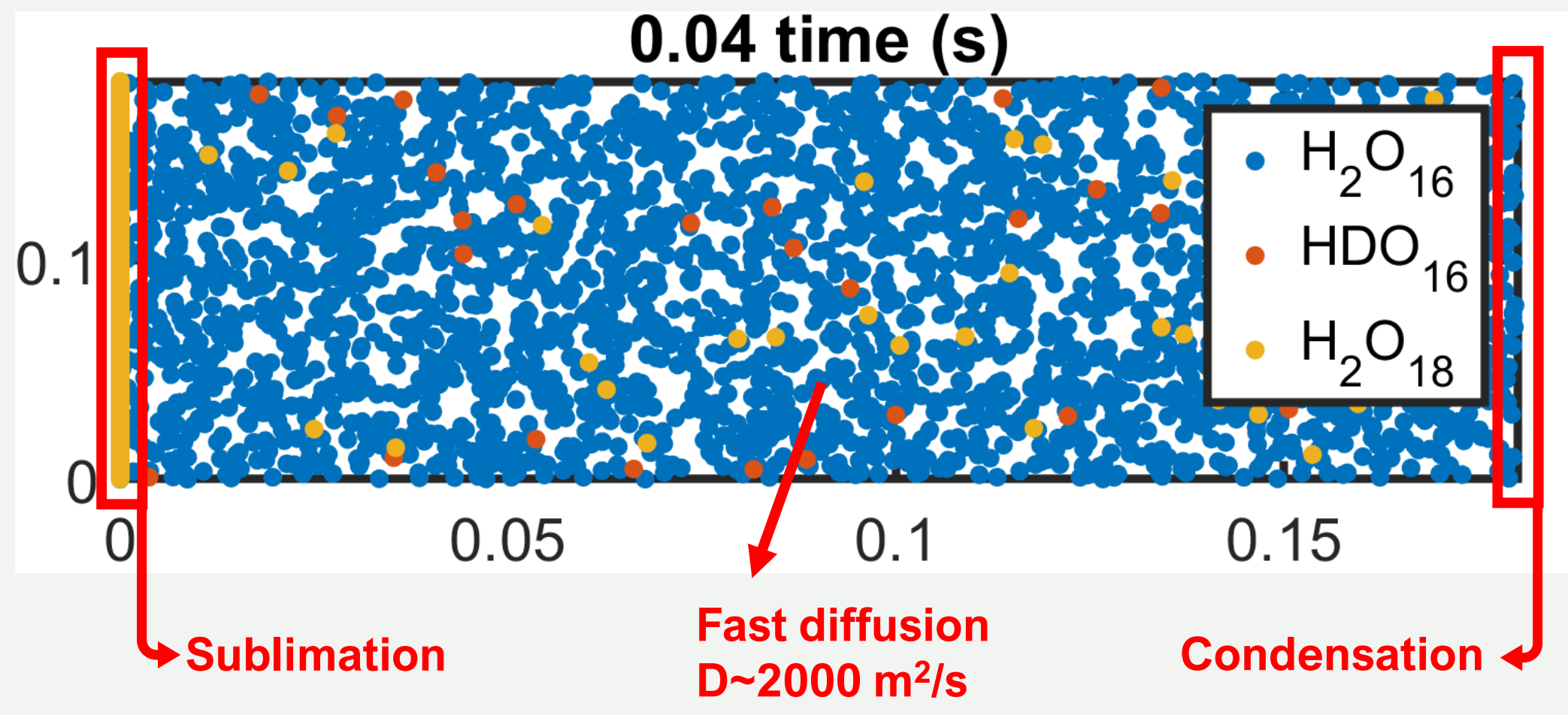
(Maxwell-Boltzmann's speed distribution)

$$f(v_{Boltz}) * dV = \frac{4}{\sqrt{\pi}}\left(\frac{m_i}{k_b T}\right)^{\frac{3}{2}} v^2 * dV * e^{-\frac{mv^2}{2k_bT}}$$

Step 3: Particle and Pressure fields

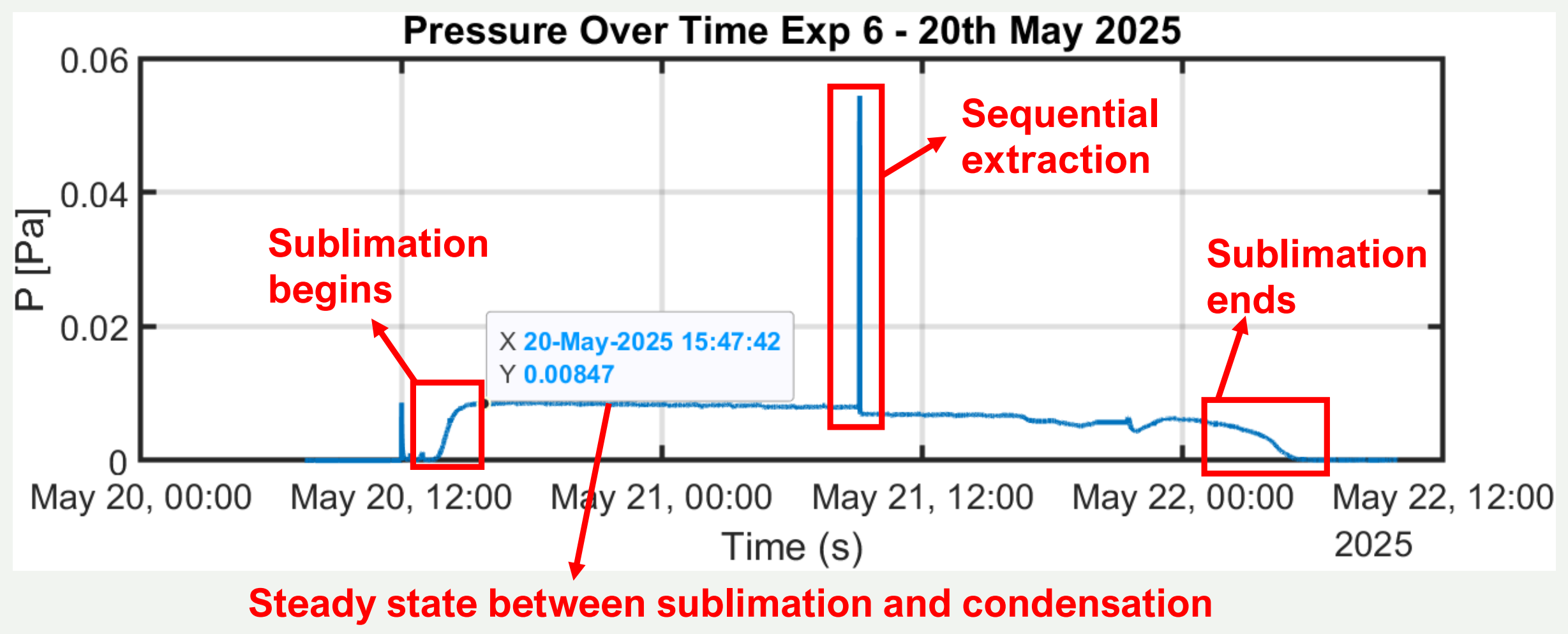


P_{total} = 0.006 Pa to 0.01 Pa

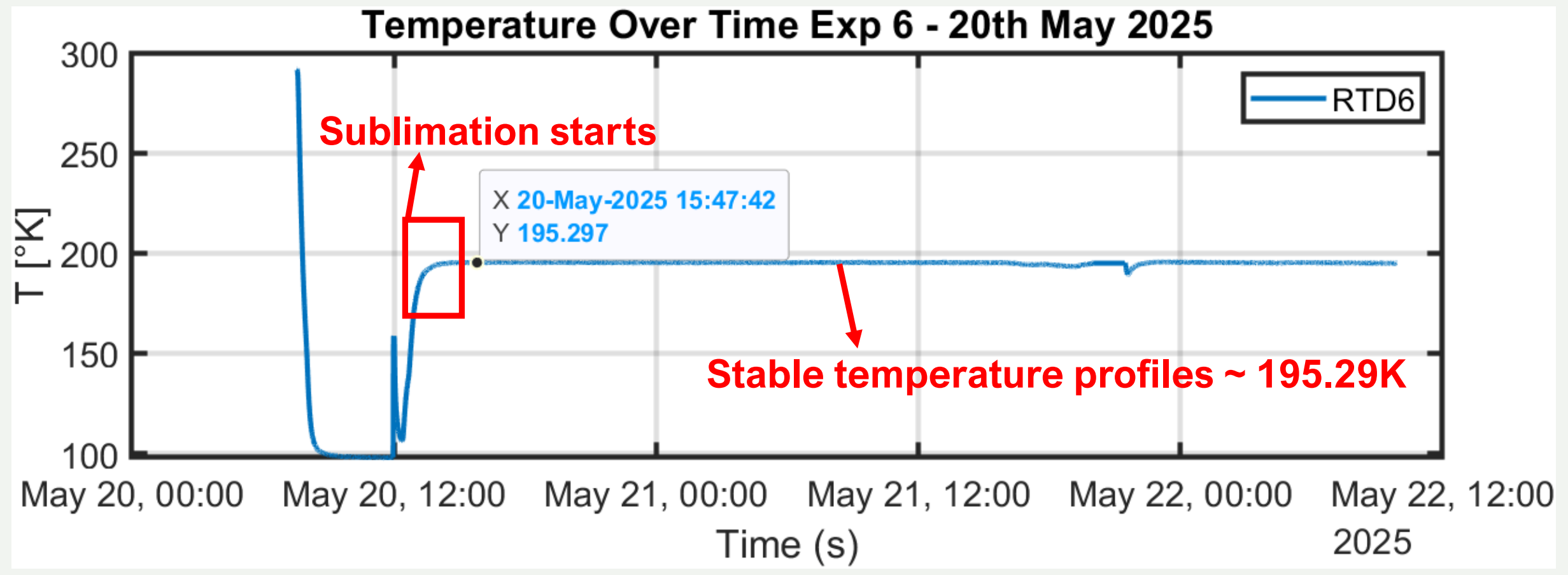


5. Results

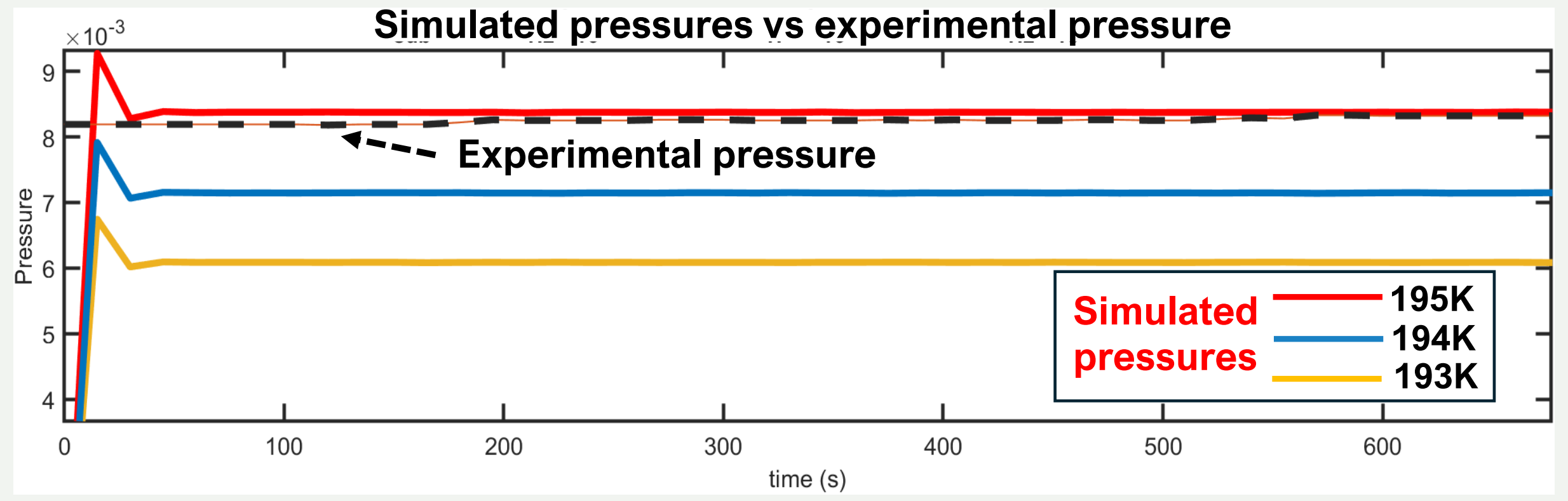
Experimental Pressure → **~ 0.008Pa at 195.29K**



Experimental Temperature → **~ 195.29K**



Simulation Pressure → **~ 0.008 Pa at 195K**



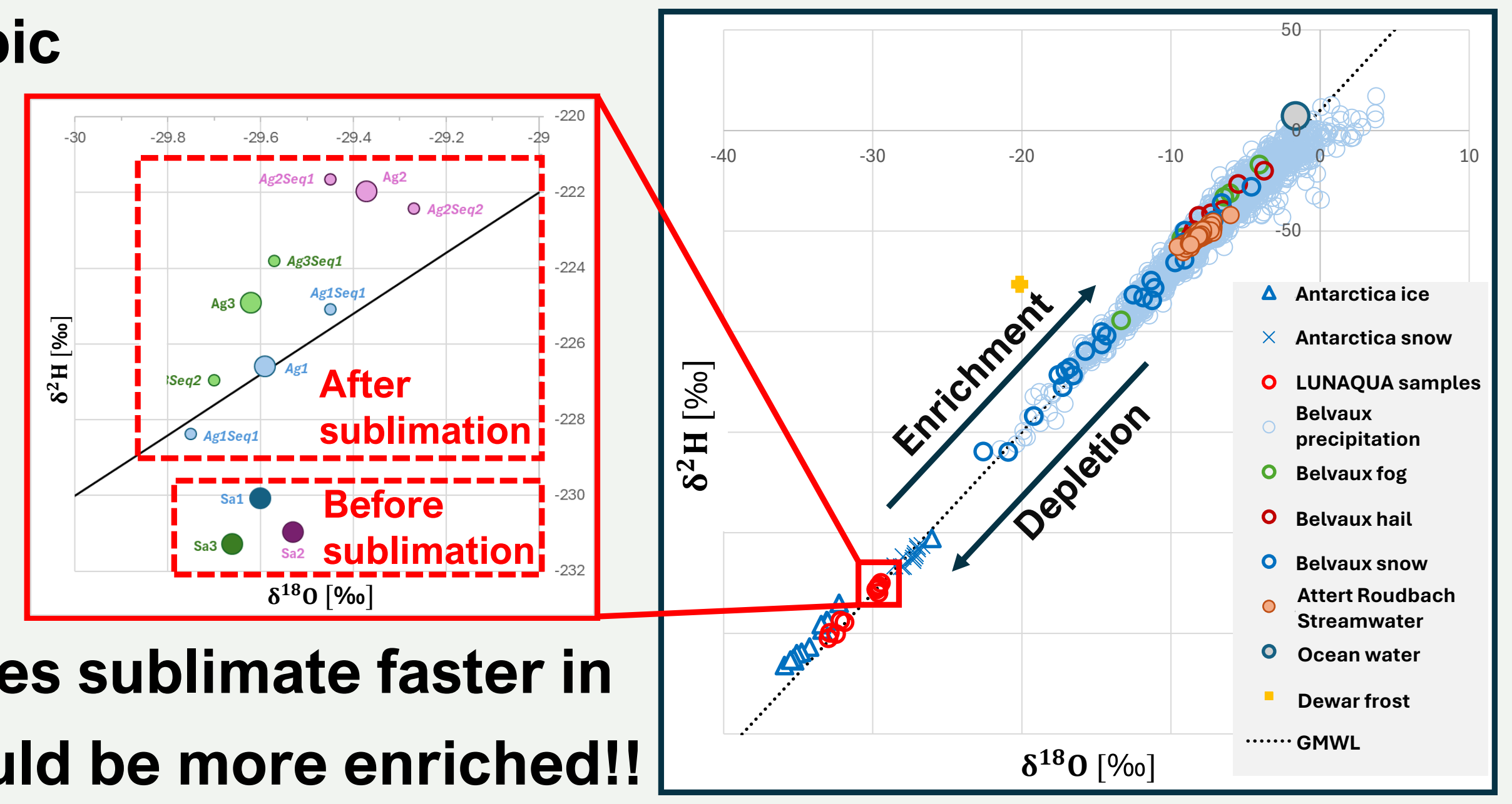
Experimental Isotopic Fractionation

2 observations:

$\delta_{Sequence1} > \delta_{Sequence2}$

1 observation:

$\delta_{Sequence1} < \delta_{Sequence2}$



Lighter isotopologues sublimate faster in 1st half; 2nd half should be more enriched!!

6. Take Aways & Outlook

1. Sublimation rates and vapor pressures are highly **sensitive** to **T_{sub}**.
2. Simulational and experimental **pressure matching** is fundamental to finally simulate isotopic fractionation (**Kinetic Gas Theory**).
3. Further experiments will collect more **isotopic fractionation evidence** to establish certainty; but fractionation can be observed.
4. Further simulations will be to find the molecular origins of **isotopic fractionation factor (α_{sub})**.