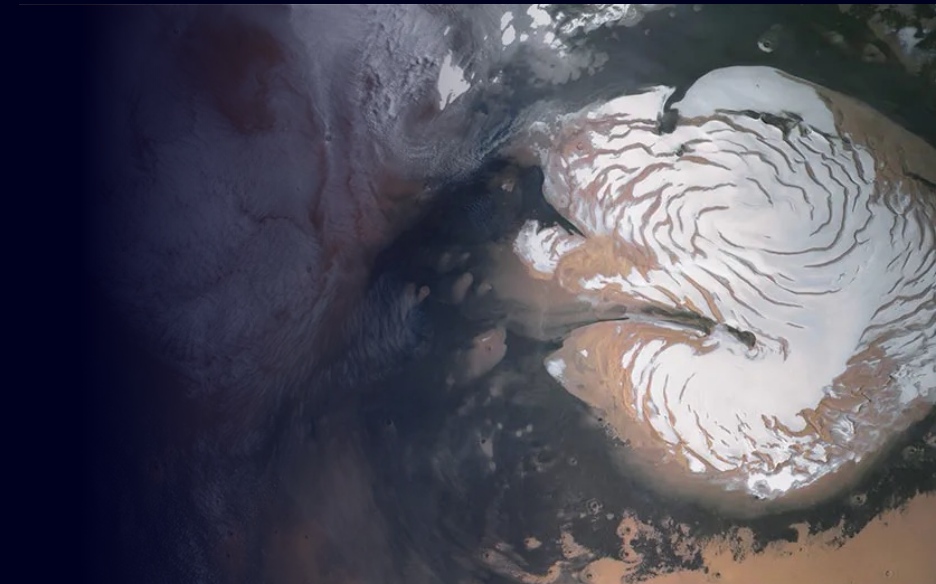


Towards Ranked Impurity Inventories of Water Resources on the Moon and Mars

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and Mars water workshops



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ESRIC-ESA workshops

Baselines for water ISRU on Moon and Mars

Webinars on 26 & 27 February 2024, follow-up at SRW 2024

Physical state

Grades/
concentrations

Impurity types and
concentrations

Focussing on the qualities of water occurrences rather than on deposit sizes and tonnages:

- How would impurities interact with ISRU technologies and add constraints to purification technologies?
- How would impurity concentrations impact our identification of economically viable resources?

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Introduction

Constraints on water purification architectures

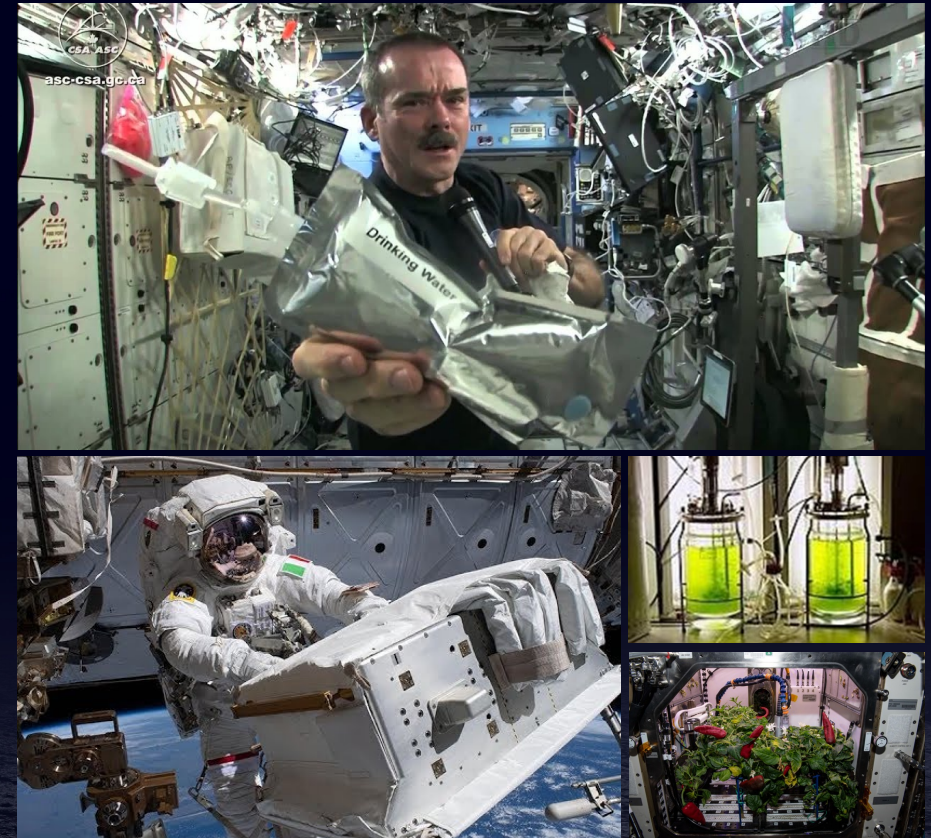
Water impurities are downstream risks

ECLSS (e.g., NASA SWEGs)

- Acute or chronic chemotoxicity
- Undesired microbiological nutrition
- Olfactory discomfort (reduced consumption)
- ...

Space/ISRU systems

- Material corrosion/degradation
- Loss of performance/reliability
- Undesired reaction products
- ...



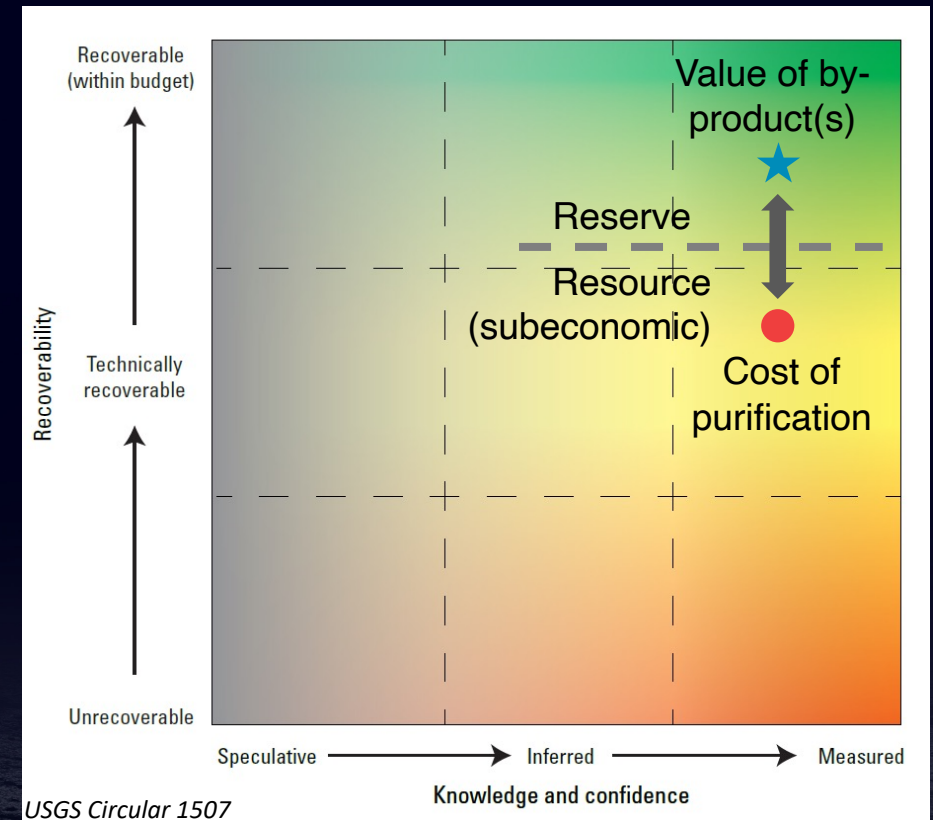
Introduction

Constraints on water purification architectures

Impurities are potential drivers into or out of economic viability

By-product recovery reward

- Geochemically limited elements (e.g., C and N)
- Energetically favourable by-products (e.g., H₂ and O₂)
- Speciality by-products, propellants (e.g., noble gases)
- ...



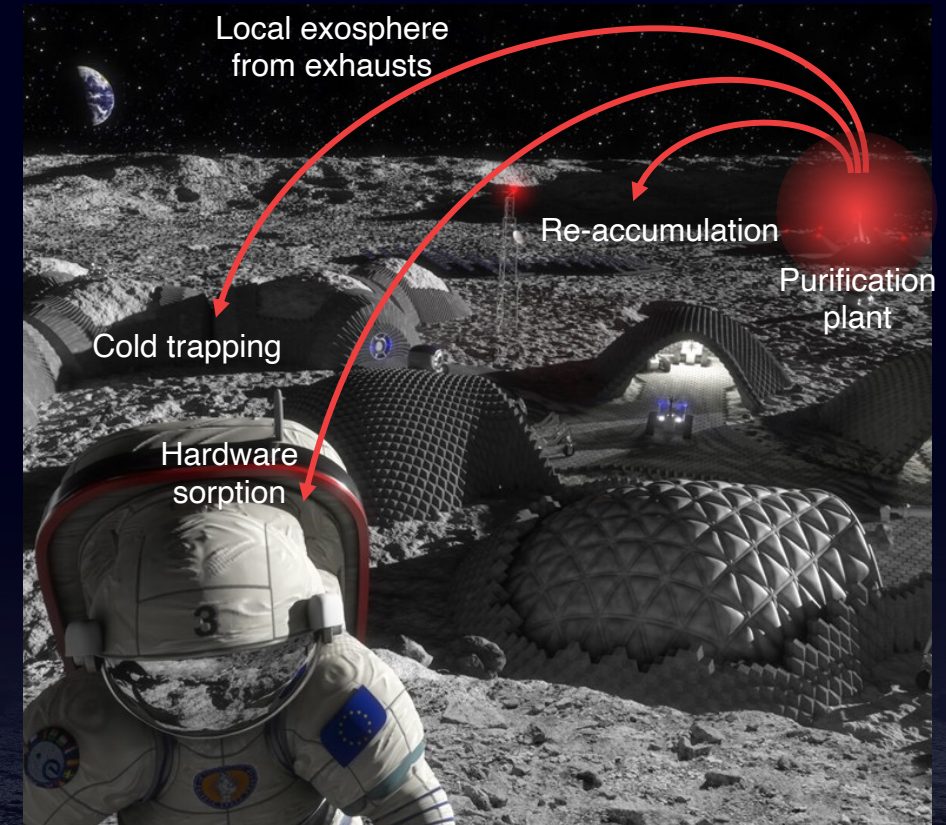
Introduction

Constraints on water purification architectures

Impurity disposal may impact the local infrastructure and environment

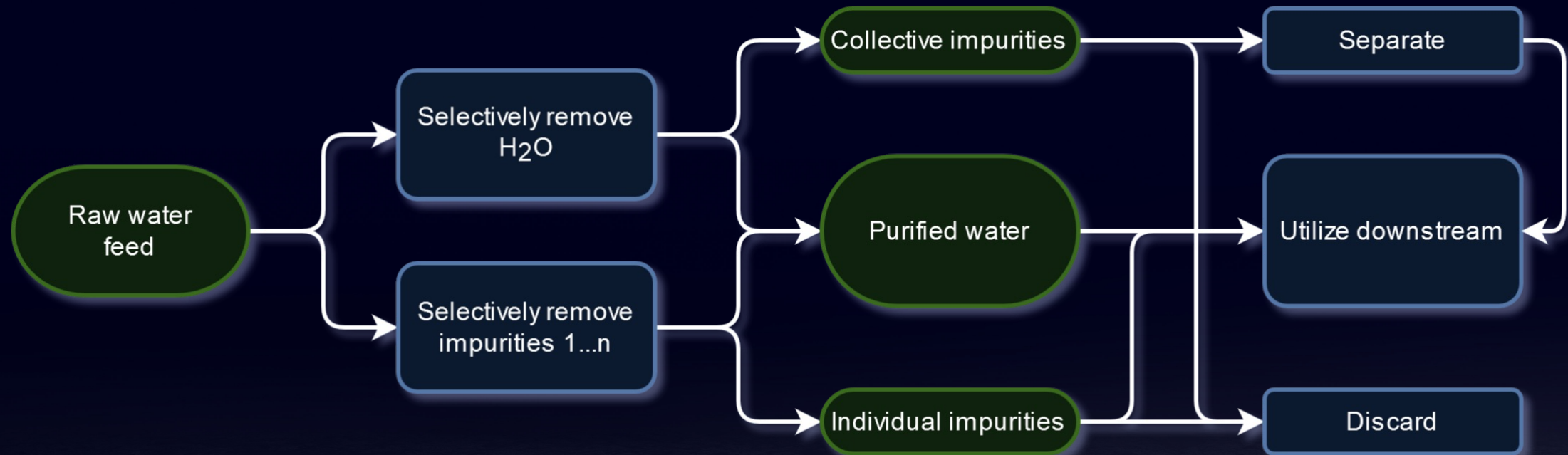
Disposal risk

- (Re-)Accumulation in cold traps
- Sorption to infrastructure and EVA hardware
- Planetary protection (e.g., niche for biological forward contamination)



Purification architectures

Selective removal of water or impurities?



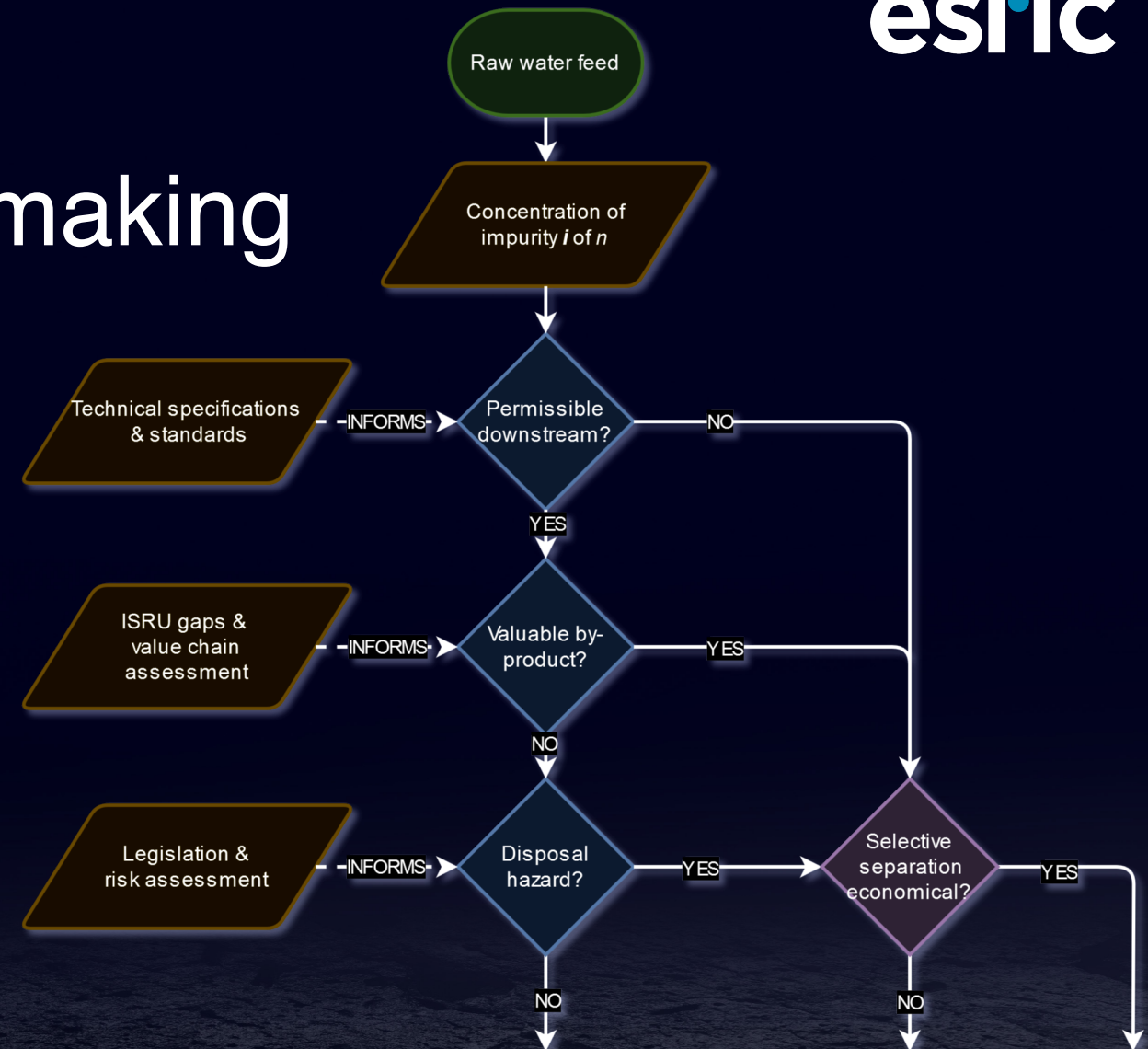
Purification architectures

Architecture decision making

Architecture decisions require iterative assessment of

- Downstream severity
- By-product value
- Disposal risks

► “Ranking” of impurity species and concentrations



Impurity tables

Pathway	Impurity species	Abundance in the effluent (influent to purification)	Downstream impact severity	Environmental disposal risk	By-product recovery reward
Evaporation, melting, calcination... (gas, liquid)			High: Hazardous		High: Very useful
			Medium: Acceptable		Medium: Niche use
			Low: No problem		Medium: Useless

Mode of extraction and physical state	Species expected as the result of extraction	Concentrations expected as the result of extraction	Negative drivers	Positive driver
			Incentive for selectively separating an impurity	

Water occurrences considered

Moon



Hydrogen in global/
circumpolar regolith



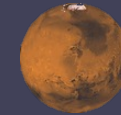
Water in pyroclastic
units



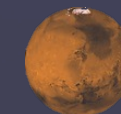
Ice in permanently
shadowed regions

LWIMS (NASA)

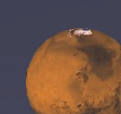
Mars



Water Trace components
in the atmosphere



Ices at polar and
mid/low latitudes



Hydrated lithologies
and regolith

M-WIP (NASA), SWIM, I-MIM (NASA), ARMADILLO (ESA)

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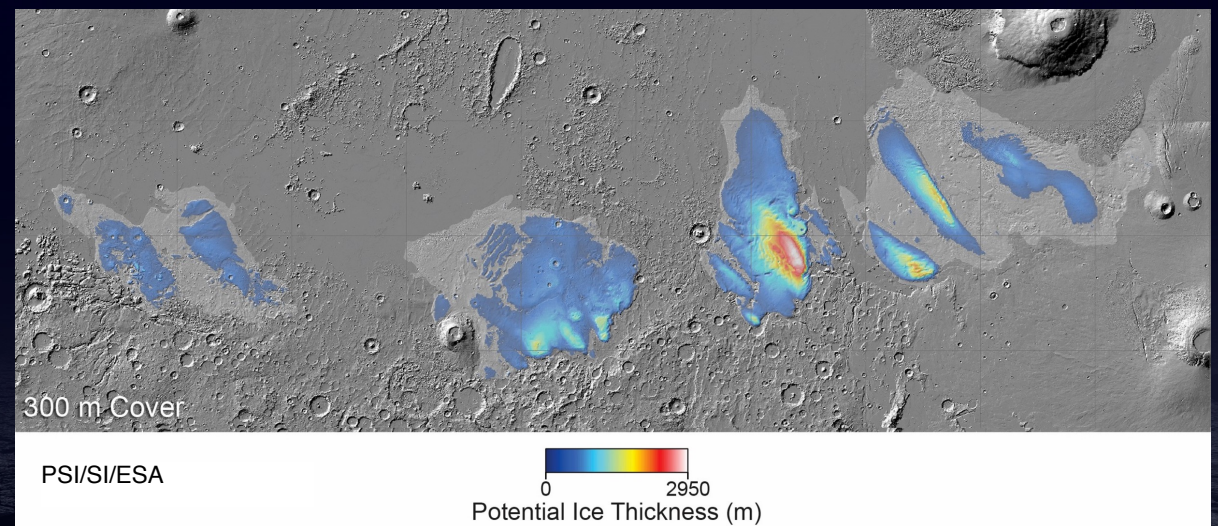
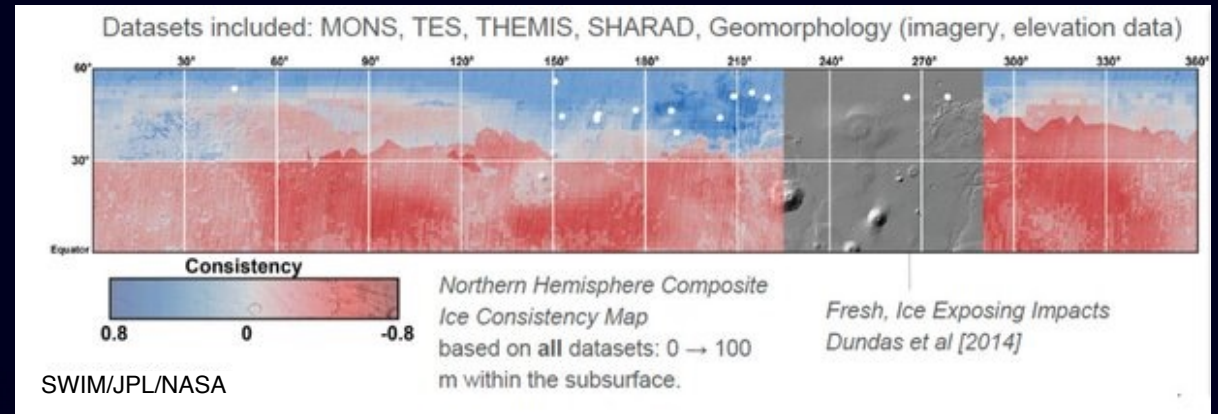


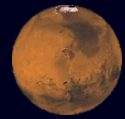
Ices at polar and mid/low latitudes

- Polar caps
- Periglacial ($>60^\circ$)
- Mid-latitude ($<60^\circ$)
- Low-latitude (Medusae Fossae Fm.)

Impurities delivered by atmospheric chemistry/dust and volcanism

- Is deposition age relevant for prediction?





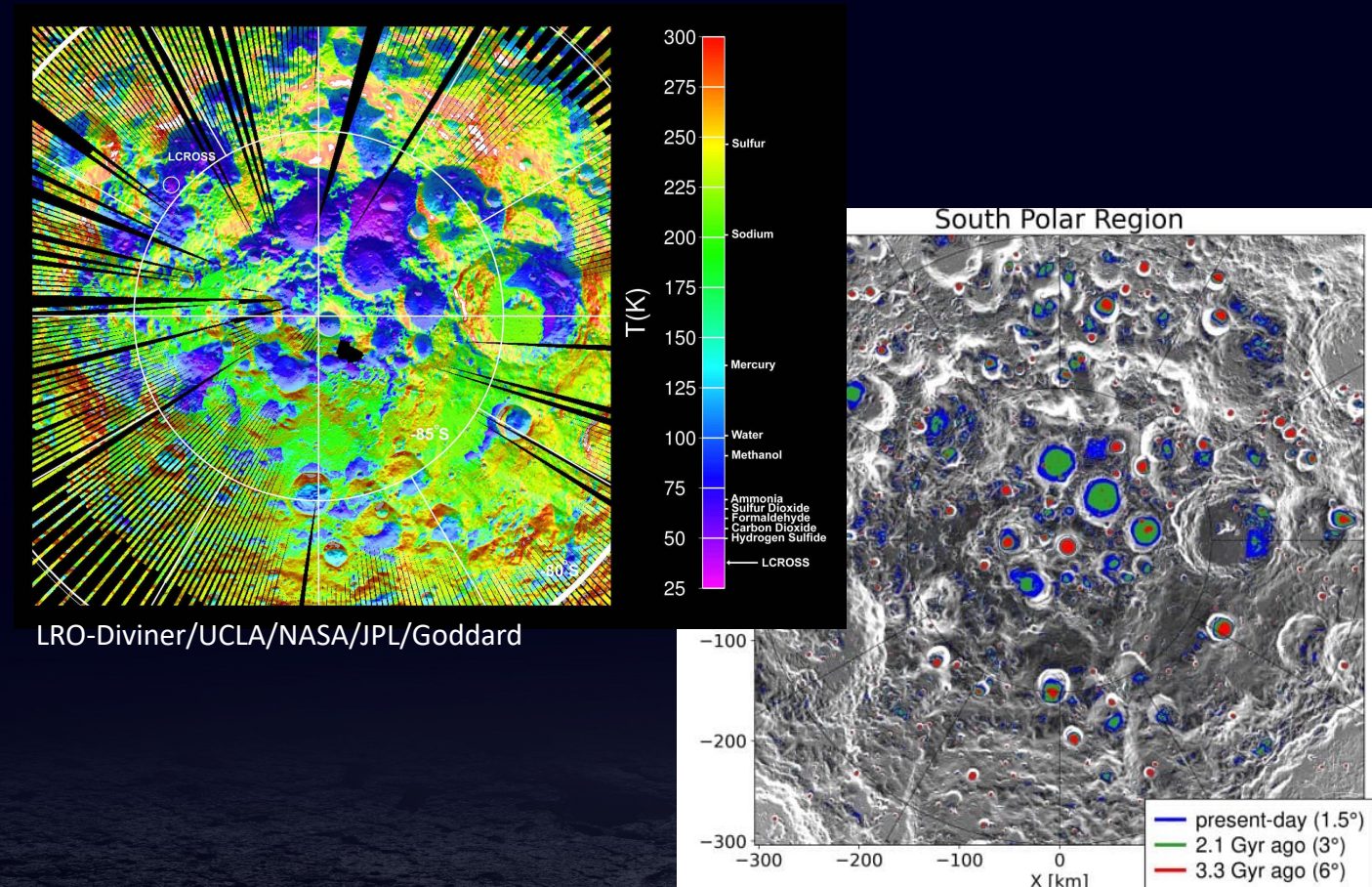
Ices at polar and mid/low latitudes

Extraction pathway	Impurity species	Estimated abundance in extraction effluent	Downstream severity	Disposal risk	Recovery reward
Evaporated ice	H ₂ S	? (deposition timing relative to volcanism)	High	Medium	Low
	HCl, HF	? (deposition timing relative to volcanism)	High	Medium	Low
	H ₂ O ₂	? (deposition timing relative to oxidizing atm. chemistry)	Medium	Low	Medium
	CO ₂	<10 mol% (more if atm. carrier gas or clathrates)	Low	Low	Low
Melted ice	ClO ₄ ⁻	<16 g/L (30 vol% initial ice)	High	Low	High
	HCl, HF, H ₂ S/H ₂ SO ₄	? (deposition timing relative to volcanism)	High	Medium	Low
	Dust	5...50 vol%	High	Low	Low
	Fe ²⁺ , Mn ²⁺	? (probably low, mostly insoluble Fe ³⁺)	Medium	Low	Low
	Mg ²⁺ , Ca ²⁺ , Na ⁺	<5 g/L	Medium	Low	Medium
	H ₂ O ₂	? (deposition timing relative to oxidizing atm. chemistry)	Medium	Low	Medium
	SO ₄ ²⁻ , Cl ⁻	<9 g/L	Medium	Low	Low
	CO ₂ , HCO ₃ ⁻	? (if clathrates present)	Low	Low	Low

Mars Phoenix WCL data and a lot of assumptions

Ice in lunar PSRs

- **Sources:** Cometary/asteroidal impactors vs. volcanic outgassing
- **Delivery:** Modification (impact, photo-/radiolysis, ...)
- **Trapping:** Fractionation through T gradients and temporal variations



Schörghofer & Rufu (2023)



Ice in lunar PSRs

Extraction pathway	Impurity species	Estimated abundance in extraction effluent	Downstream severity	Disposal risk	Recovery reward
Heating and evaporation (low-T gas)	NH ₃	0.5...6 mol%	High	Medium	High
	H ₂ S	2...16 mol%	High	High	Medium
	Hg	<0.6 mol% (0.4 wt% in PSR soil)	High	High	Low?
	HCHO, HCN, COS, CS ₂	? (expected in cometary source)	High?	High?	Low?
	HCl, HF	? (expected in volcanic source)	High?	High?	Low
	CH ₃ OH	<8 mol% (high uncertainty)	High	Medium	High
	SO ₂	<3 mol%	High	Medium	Low?
	CO ₂	<5 mol%	Low	Low	High
	CO	<4 mol%	Medium	Low	High
	C ₂ H ₄ (CH ₄ , C ₂ H ₆)	<5 mol%	Medium	Low	High
	H ₂	<9 mol% (high uncertainty)	Low	Low	High

LCROSS data and a lot of assumptions

Conclusions

Baselines for water ISRU

Impurity types and concentrations

Decisions on purification architectures hinge on:

- Impurity inventories and extractive modifications
- Downstream requirements and environmental risks
- By-product value and economic viability of recovery

More data needed on lunar and Martian ices:

- Fundamental scientific understanding of water cycles
- Predictive genetic modelling of deposits for ISRU architectures