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LUNAR RESOURCES

NASA

THERMOCHEMICAL MODELING OF MOLTEN REGOLITH ELECTROLYSIS SUPPORTING ASSESSMENT OF METALLIC PRODUCT COMPOSITIONS AND DYNAMIC OXIDE PROPERTIES

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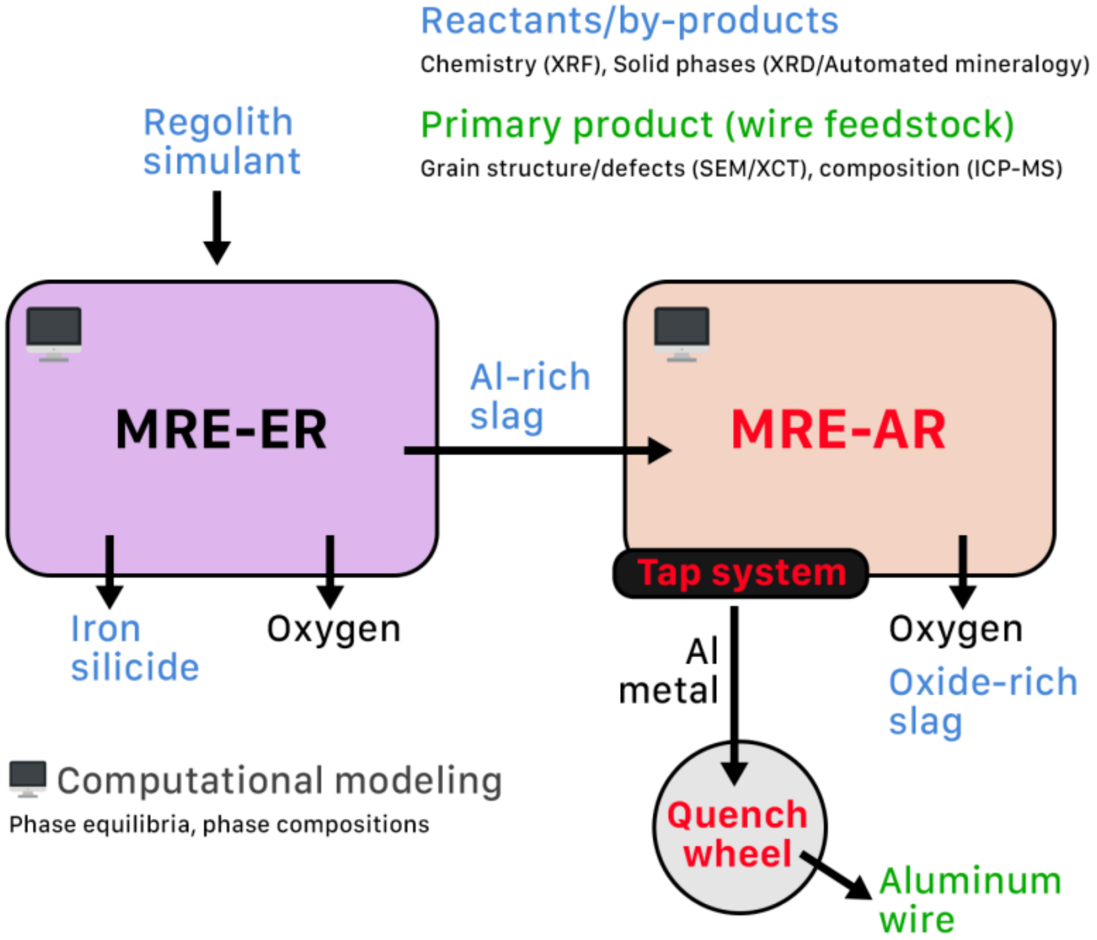
SPACE RESOURCES ROUNDTABLE
June 3-6, 2025

Background – MAGMA Project

Project Goal: Produce additively manufacturturable aluminum from lunar regolith



Aluminum from Regolith: Composition Considerations

Wrought Aluminum Alloys

	Alloy Series	Primary Alloying Additions
	1xxx	None
HT	2xxx	Copper **(Absent from regolith)**
	3xxx	Manganese **(Present in regolith)**
	4xxx	Silicon **(Present in regolith)**
	5xxx	Magnesium **(Present in regolith)**
HT	6xxx	Mg + Si **(Present in regolith)**
HT	7xxx	Zinc **(Absent from Regolith)**
	8xxx	Lithium, Others **(Absent)**

Cast Aluminum Alloys

Alloy Series	Primary Alloying Additions
1xx.x	None
2xx.x	Copper **(Absent from regolith)**
3xx.x	Si + Cu **(Absent from regolith)**
4xx.x	Silicon **(Present in regolith)**
5xx.x	Magnesium **(Present in regolith)**
6xx.x	**Unused designation**
7xx.x	Zinc **(Absent from Regolith)**
8xx.x	Tin **(Absent from regolith)**

HT = Heat Treatable for Strengthening

Other Regolith Elements: **Ca**, Na, Fe, K, Ti, P **(Contaminants?)**

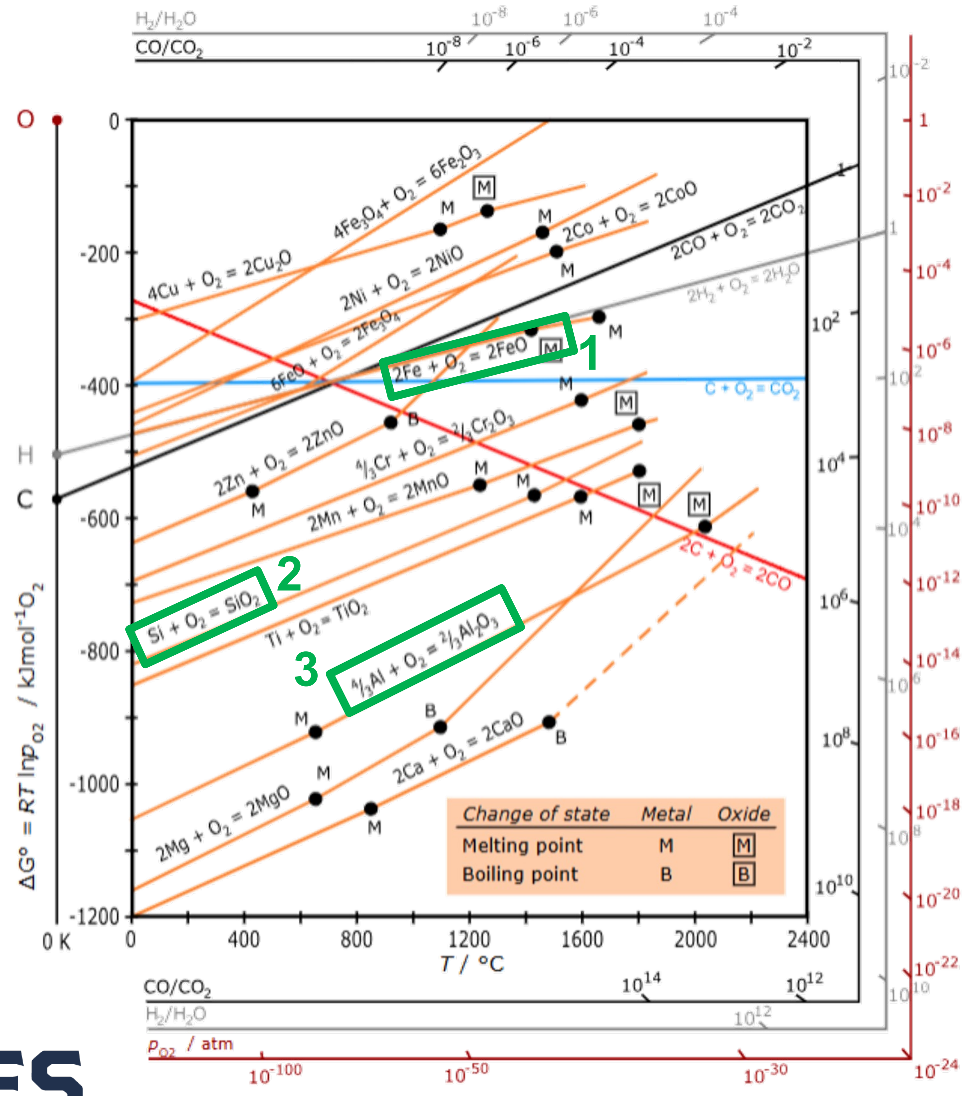
Ref: ESAB, "Understanding the Aluminum Alloy Designation System," 2021

Role of Thermochemical Modeling in FactSage

1. Estimate achievable product metal compositions
    - **Governed by the thermodynamics of reduction processes**
2. Identify process temperature requirements
    - **Governed by the evolution of the molten oxide liquidus temperature**
3. Calculate molten oxide viscosity evolution to support outflow pathway and hardware design

Reduction of oxide species in regolith is not perfectly discrete!

Ellingham Diagram



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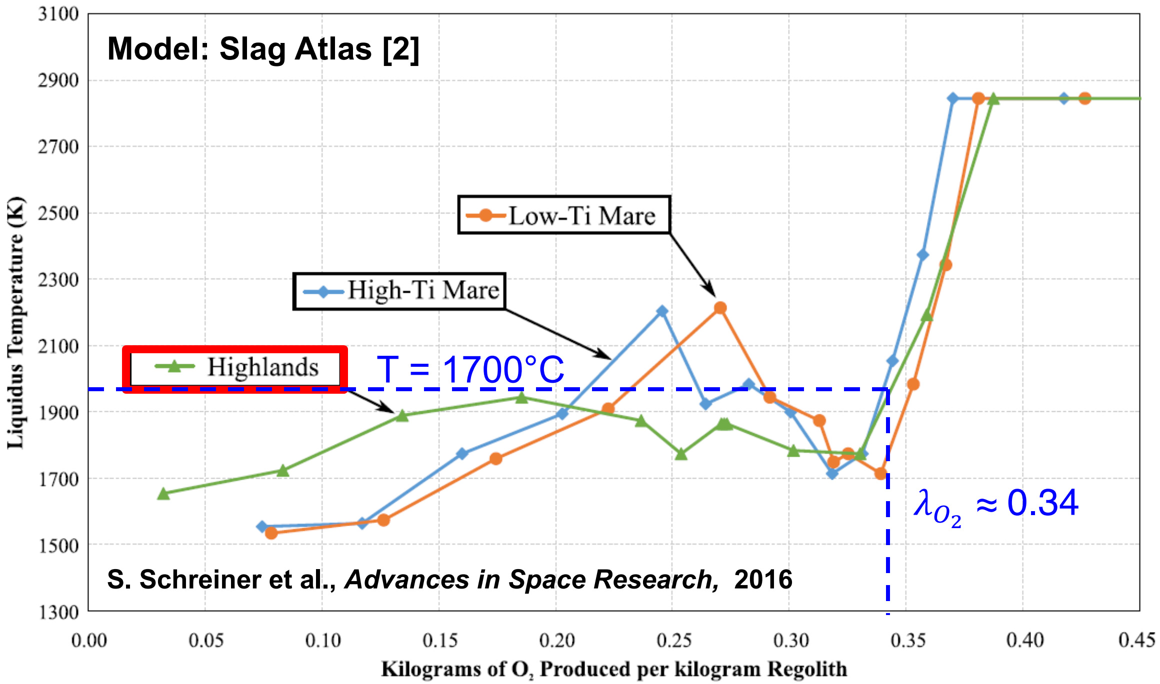

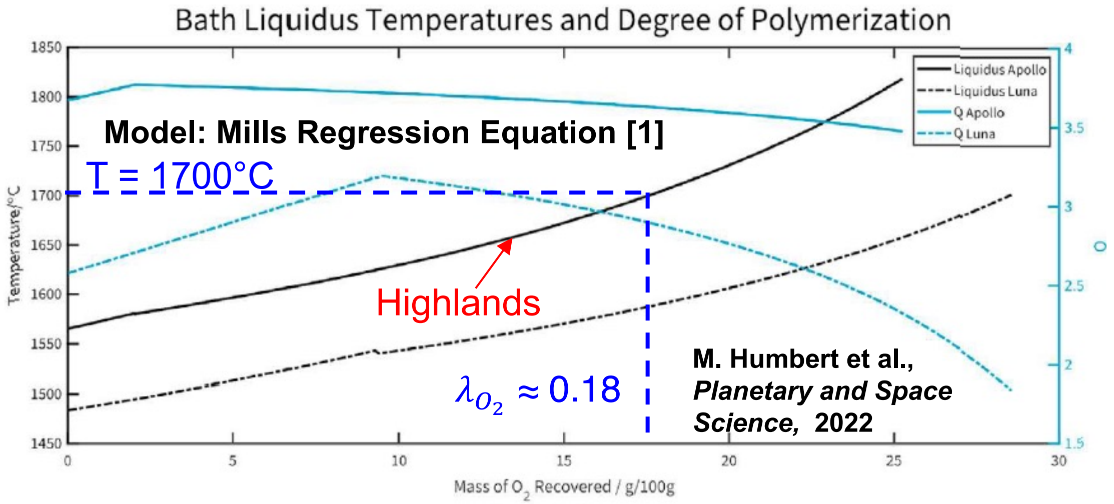

Electrolysis Reaction Progress Coordinate $\lambda_{O_2} = \frac{m_{O_2}}{M_0}$

Clarification of the liquidus evolution behavior is needed to identify temperature requirements.

[1] K.C. Mills, et al., *J. S. Afr. Inst. Min. Metall.*, 2011
[2] M. Allibert et al., Verlag Stahleisen, GmbH, 1995

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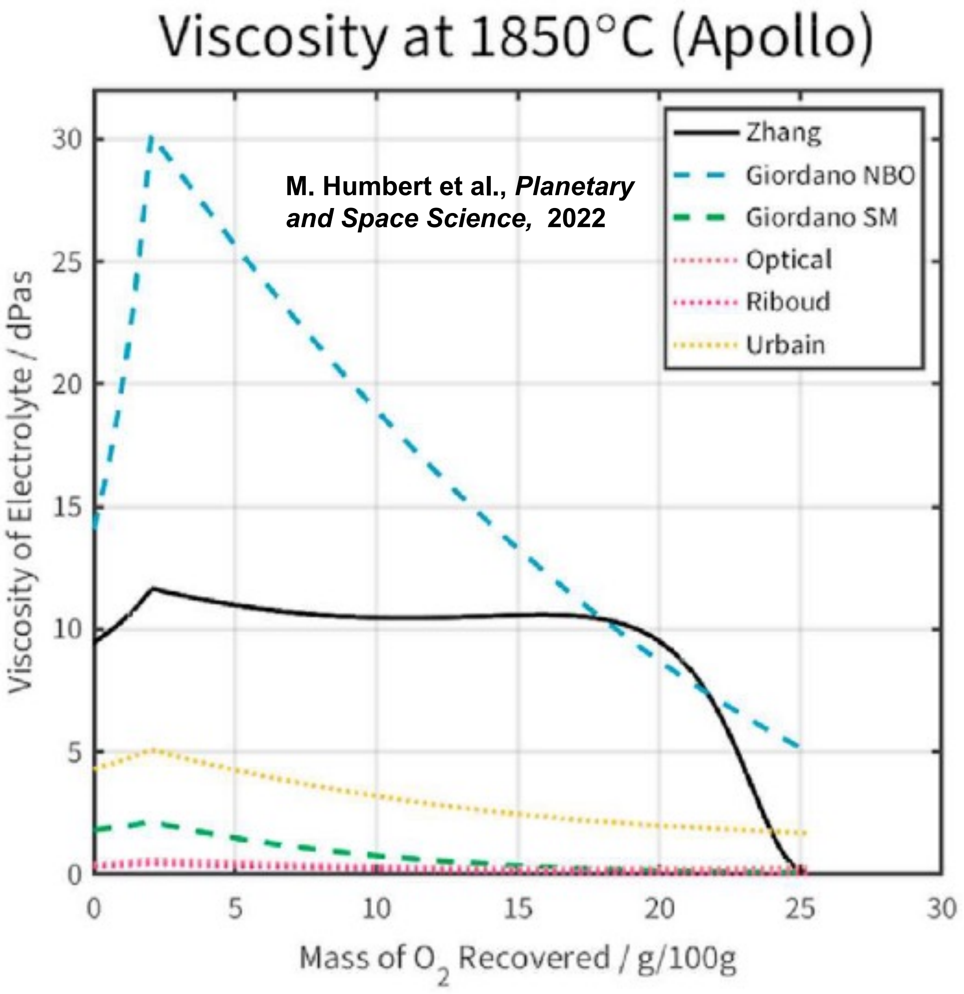
Literature viscosity models span orders of magnitude.



Model Setup & Assumptions

- **Isothermal, isobaric reactor**
  - Ultimately, T & P to match experimental conditions
- **Three perfectly separated phases**
  1. Molten Oxide: Consumed with electrolysis
  2. Metallic: Accumulates with electrolysis
  3. Gas: Continuously vented (no accumulation)
     - O2 + Metal-bearing volatiles
     - Permanently excluded from model system
- **Recursive model defines reactor contents on an incremental, stepwise basis. $\Delta(\lambda_{O_2})$ is imposed.**

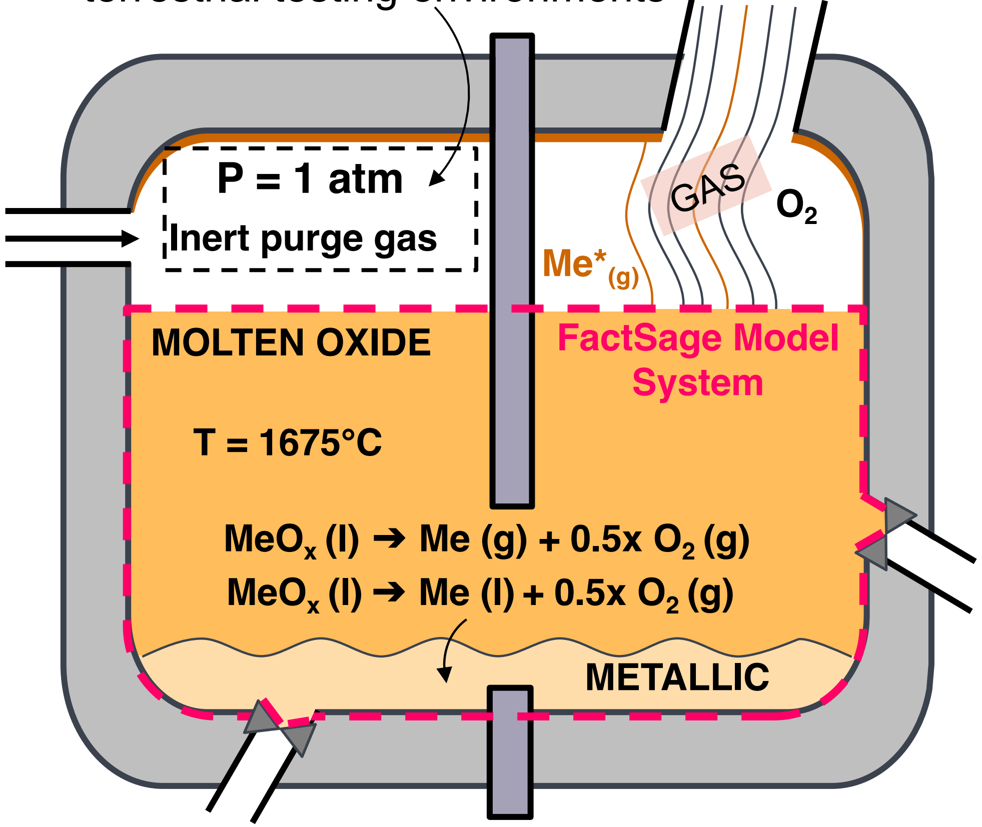
Equation for Oxygen in System

$$m_{Ox,i} = m_{Ox,i-1} - (\Delta(\lambda_{O_2})_{(i-1)\rightarrow i})M_0 - \sum_{k=1}^{N} \frac{n(MW_{Ox})}{MW_k} * m_{k,gas}$$

Equation for Metal Species in System

$$m_{Me,i} = m_{Me,i-1} - \sum_{k=1}^{N} \frac{n(MW_{Me})}{MW_k} * m_{k,gas}$$

Initial modeling case supports terrestrial testing environments



B. Schneiderman et al., *Acta Astronautica*, vol. 234, pp. 1-12 (2025)

Key Stages of Electrolysis for Metal Extraction

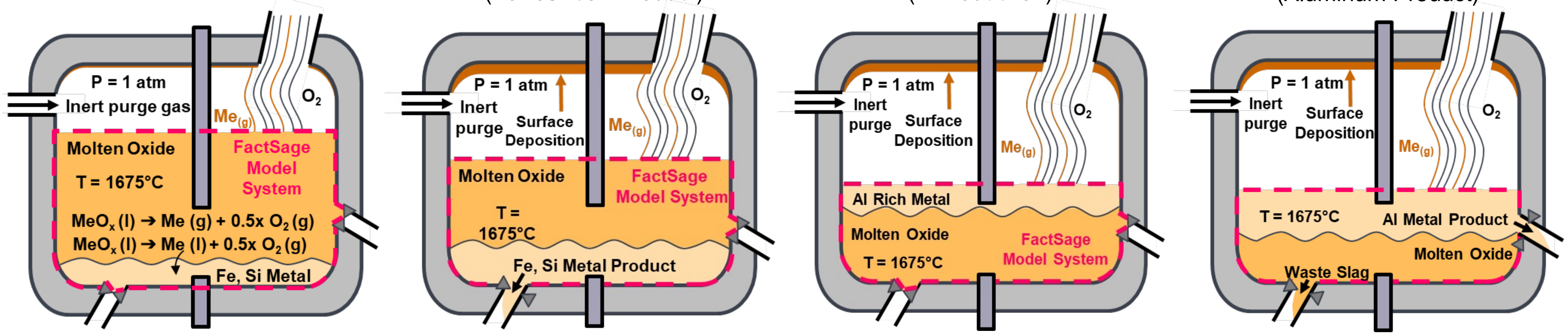
- All results assume the initial composition of the highlands simulant **CSM-LHT-1**.
- Two “Extraction Events” in model to isolate ferrosilicon and aluminum products

λ_{O_2} << 0.30:
Early-Stage Electrolysis
(Fe, Si Reduction)

λ_{O_2} = 0.30:
Extraction Event 1
(Ferrosilicon Product)

0.30 < λ_{O_2} < 0.37:
Late-Stage Electrolysis
(Al Reduction)

λ_{O_2} = 0.37:
Extraction Event 2
(Aluminum Product)

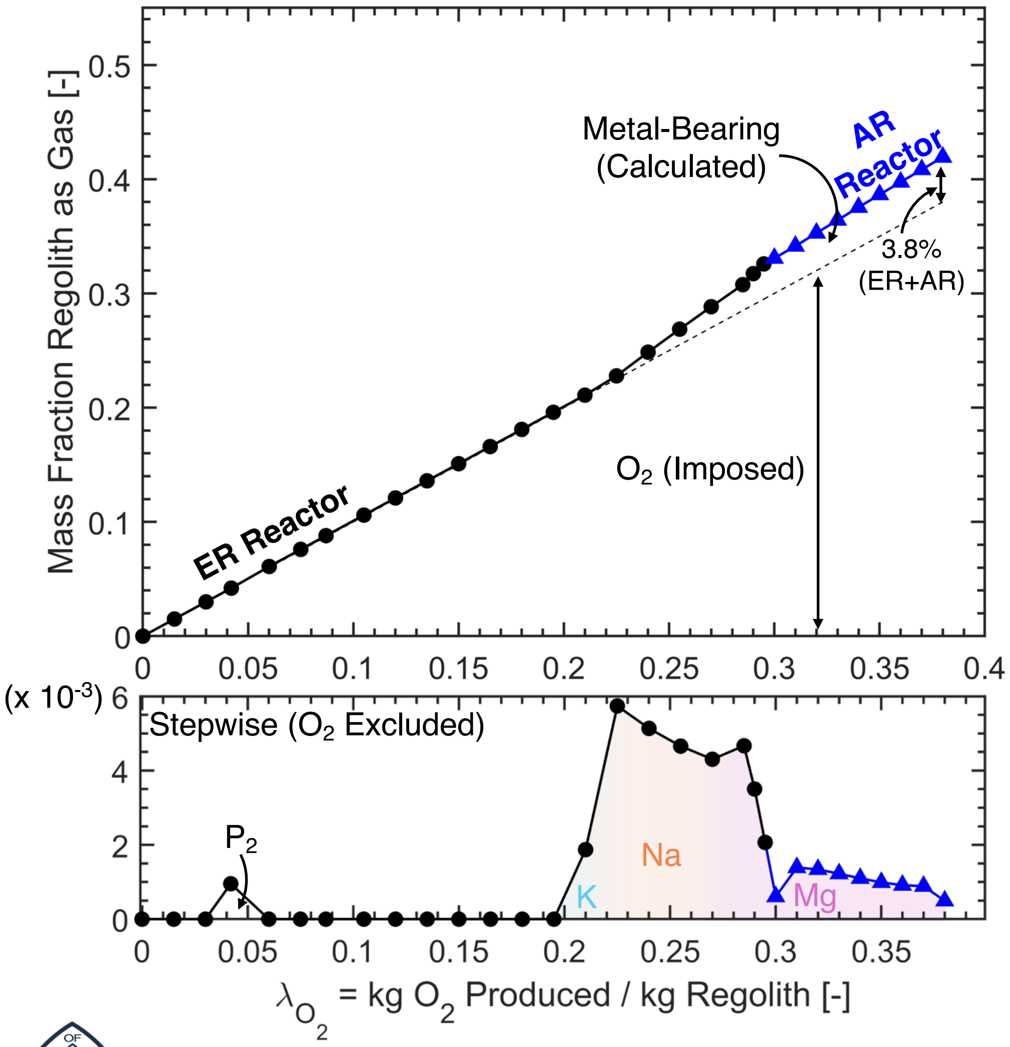


*Me(g) refers to metal-bearing gaseous species that may contain oxygen atoms also

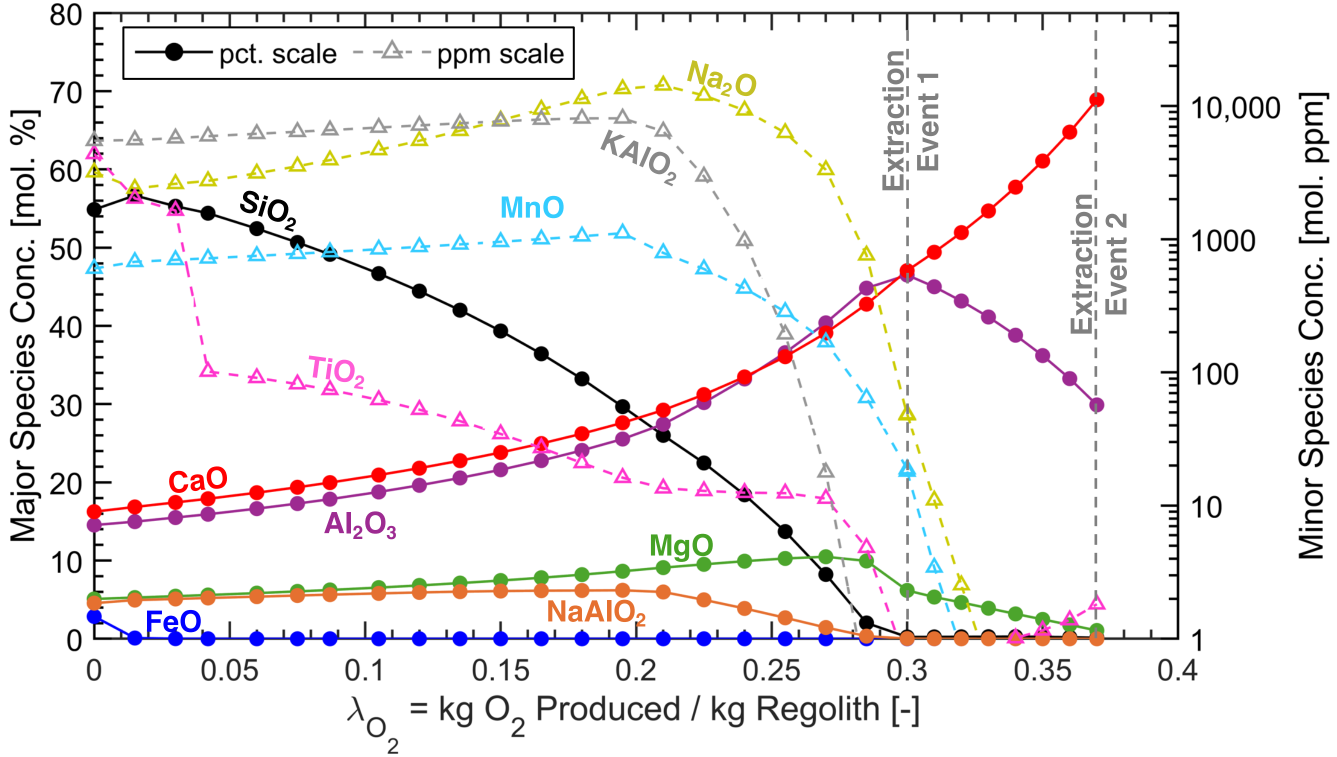
B. Schneiderman et al., *Acta Astronautica*, vol. 234, pp. 1-12 (2025)

Composition Trajectory of Each Process Stream

Gas Evolution and Composition



Molten Oxide Composition



Metal Product Compositions

[wt.%]	Si	Al	Fe	Ti	Mg	Mn	Ca
Event 1	84.75	3.09	10.99	1.13	0.0023	0.024	0.013
Event 2	0.30	99.27	-	-	0.0017	-	0.43

B. Schneiderman et al., Acta Astronautica, vol. 234, pp. 1-12 (2025)

Influence of Product Isolation Effectiveness

Literature Assumption: Perfectly Discrete Reduction:

$SiO_2 \rightarrow Si + O_2$

$Al_2O_3 \rightarrow 2\ Al + 1.5\ O_2$

$CaO \rightarrow Ca + 0.5\ O_2$

Extraction Event 1

Time and λ_{O_2} $\longrightarrow$

FactSage Model: Parallel Reduction of Dilute Species with Competing Reactions:

$SiO_2 \rightarrow Si + O_2$

Extraction Event 2 is Liquidus-Limited

$Al_2O_3 \rightarrow 2\ Al + 1.5\ O_2$

Suboptimal Extraction Event 1

$CaO \rightarrow Ca + 0.5\ O_2$

Optimal Extraction Event 1

$3\ CaO + 3\ Si + 2Al \rightarrow 3\ CaSi + Al_2O_3$

Time and λ_{O_2} $\longrightarrow$

Ca concentration depends on the amount of residual Si after Extraction Event 1

Most **Optimal** Case Model:
0.3 wt. % Ca, 0.2 wt. % Si

Suboptimal Case Model:
4.0 wt. % Ca, 2.8 wt. % Si

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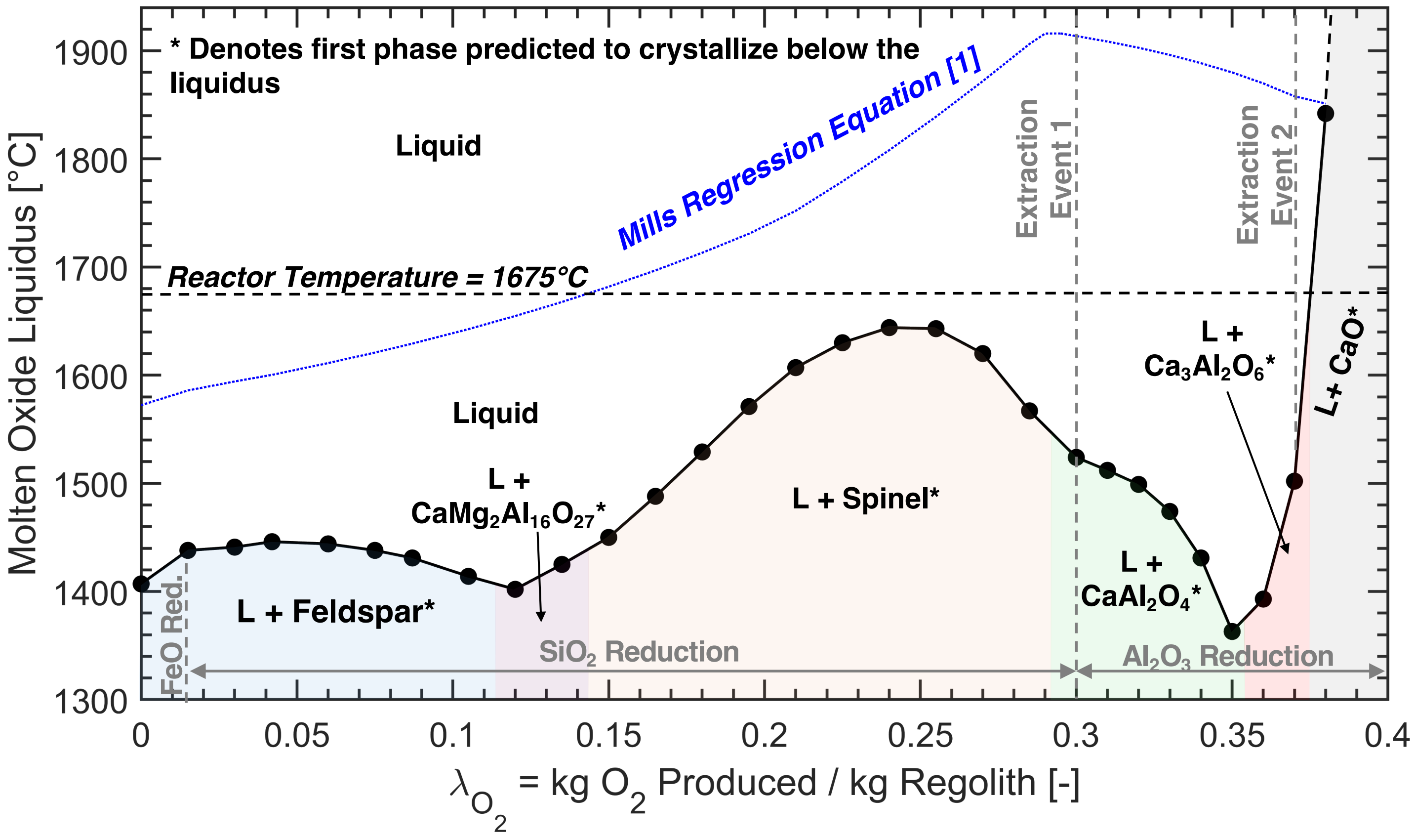
Molten Oxide Liquidus Temperature Evolution

[1] K.C. Mills, et al., *J. S. Afr. Inst. Min. Metall.*, 2011

- Wide disparity between FactSage and Mills regression equation
- FactSage reflects similar trends to the Slag Atlas, but considers all species in slag
- Operating temperature of 1675°C remains ~30°C above the intermediate maximum in liquidus
  - A more conservative safety margin may be needed



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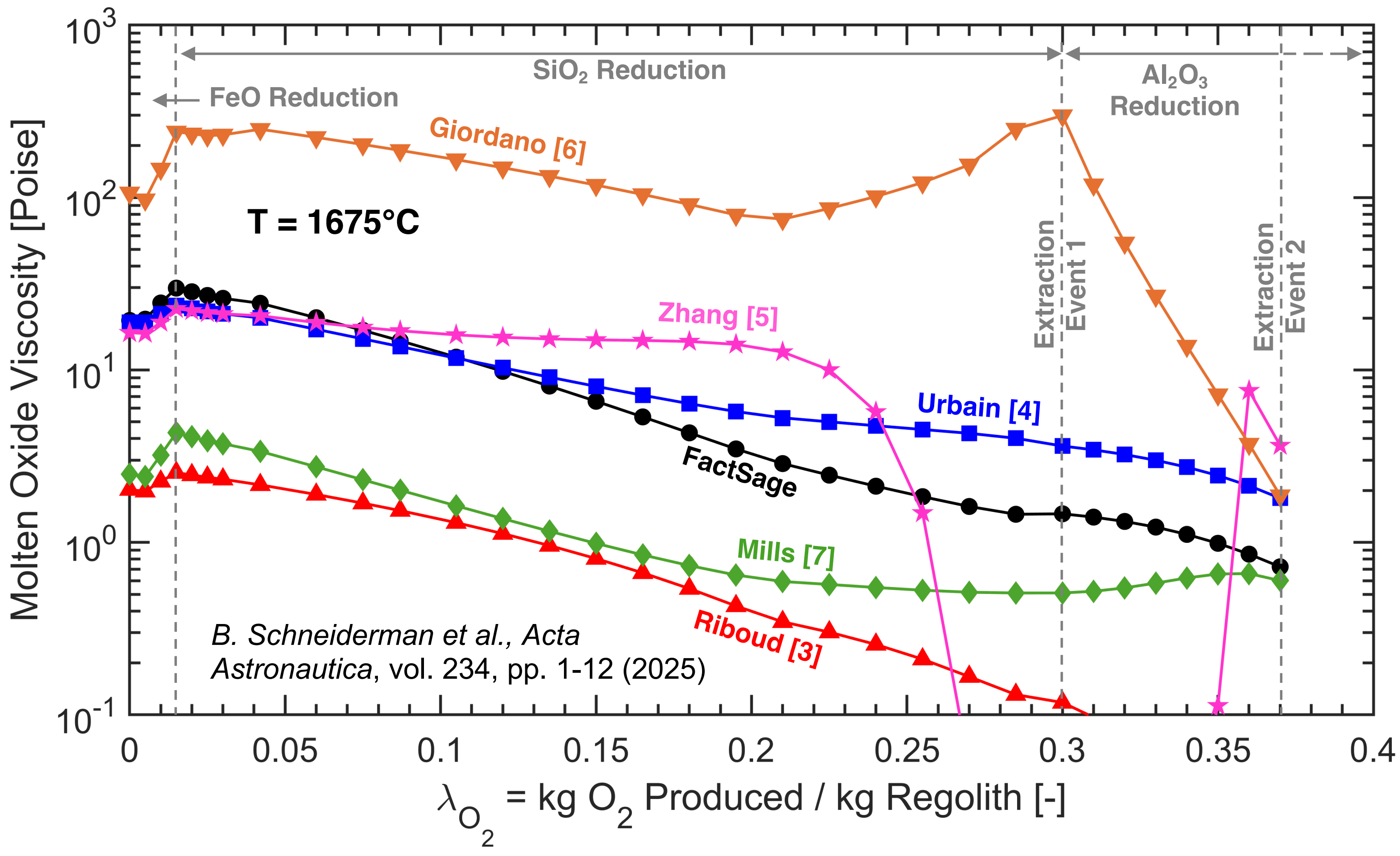
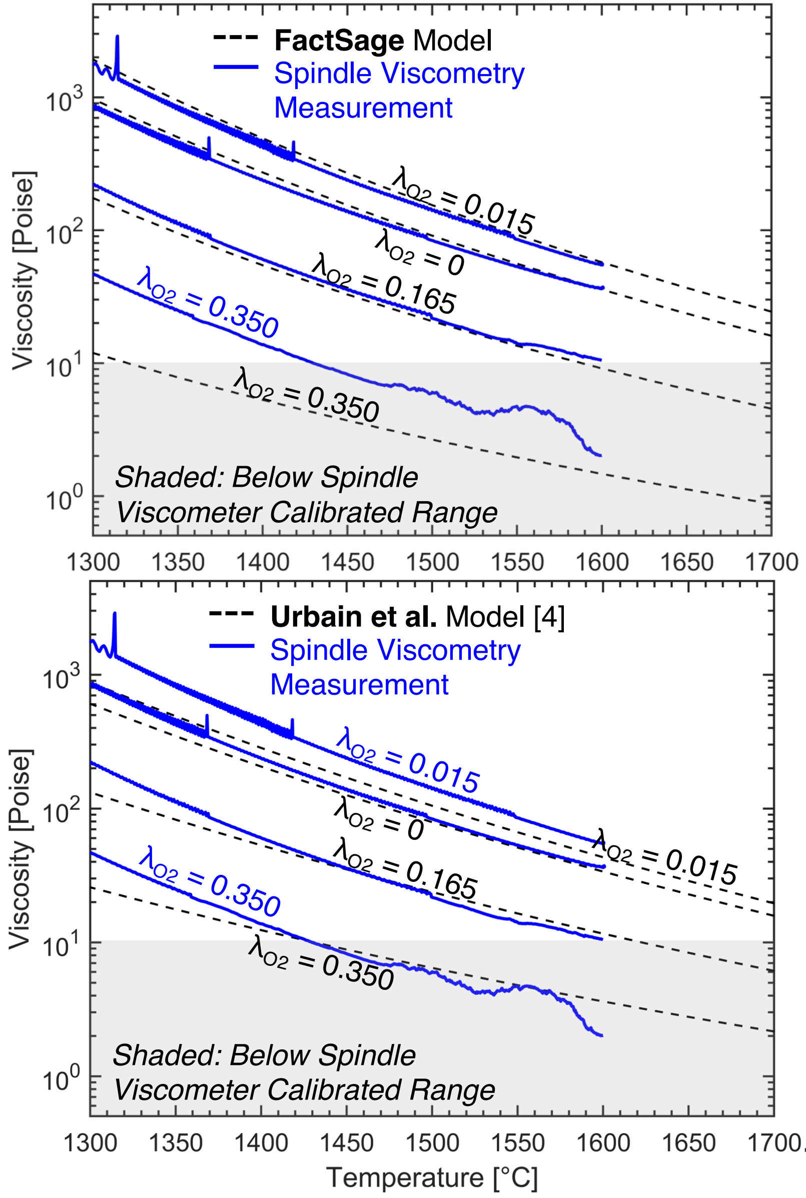
Molten Oxide Viscosity Evolution





Viscosity Model References: [3] P.V. Riboud et al., Fachber. Huttenprax. Metallweiterverarb. (1981); [4] G. Urbain et al., Geochim. Cosmochim. Acta (1982); [5] G.-H. Zhang et al., Metall. Mater. Trans. B (2012); [6] D. Giordano and D.B. Dingwell, Earth Planet. Sci. Lett. (2003); [7] K.C. Mills and S. Sridhar, Ironmak. and Steelmak. (1999)

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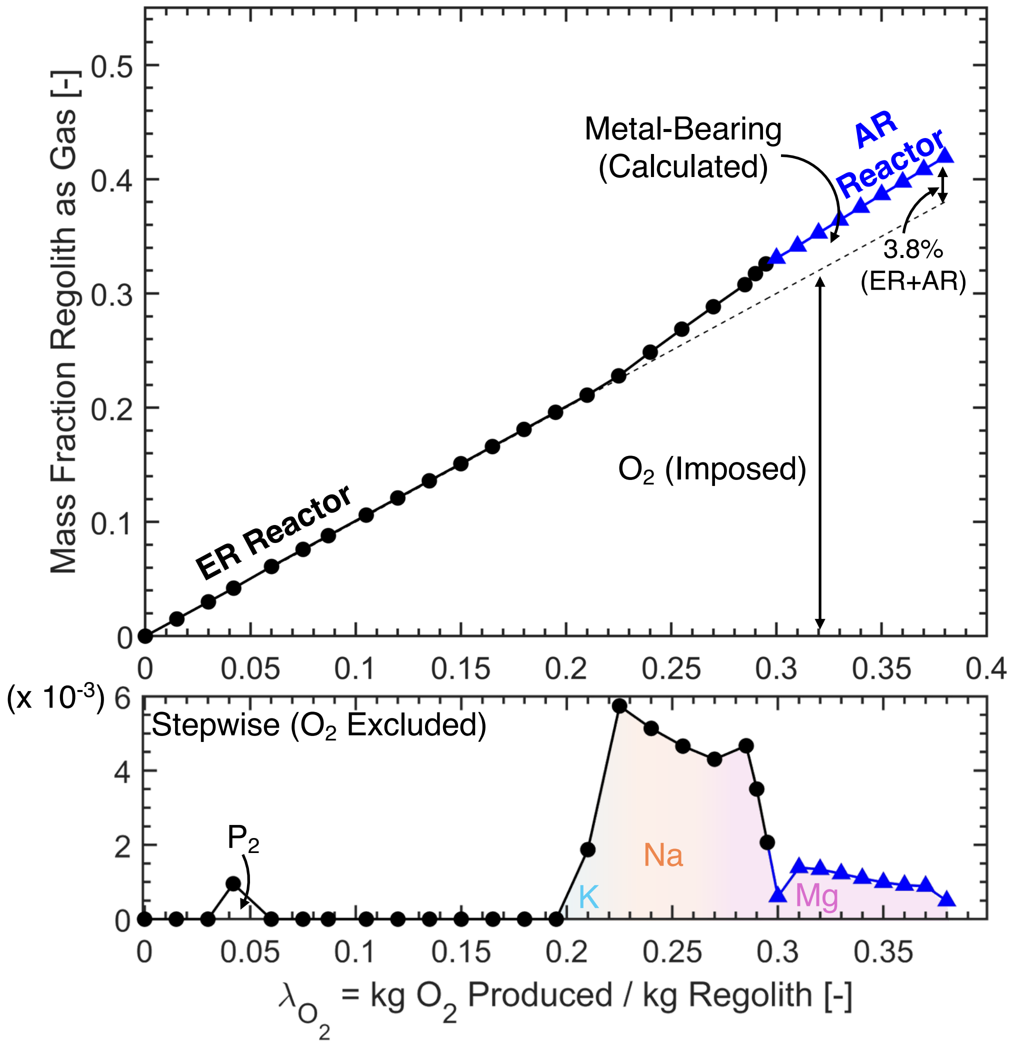
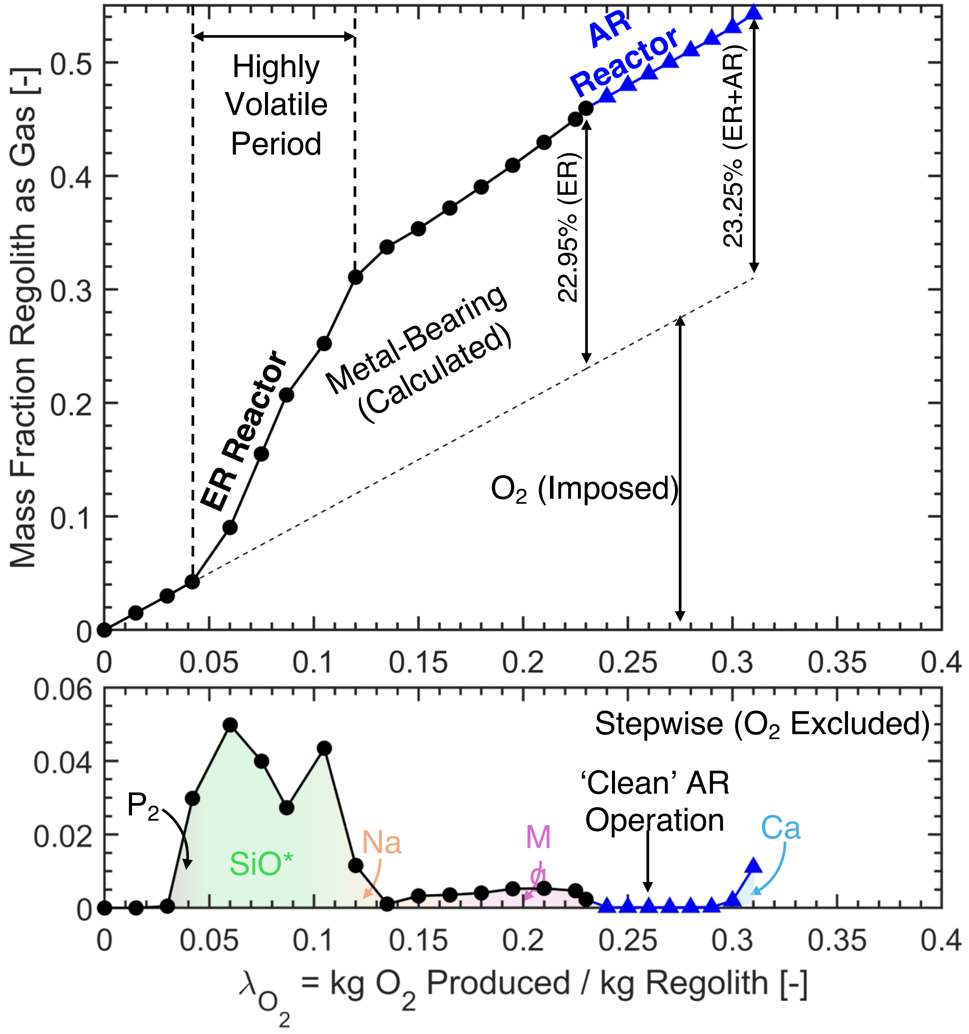
Influence of Ullage Pressure

1 atm



0.068 atm (~ 50 torr)



__Note:__ Oxygen lost to SiO is **not** counted in λ_{O_2}, causing a leftward shift of the curve in the 0.068 atm condition.

Conclusions

- Ferrosilicon and aluminum product compositions with an isolation event at λ_{O_2} = 0.30 can nearly meet those of terrestrially employed materials.
  - Ca is a potentially unavoidable alloying addition that is not commonly employed terrestrially.
    - Ca concentration depends on the amount of residual Si after “Extraction Event 1”.
  - Small amounts of Ca in cases of near-ideal product isolation still result in drawable Al wires.
- A minimum operating temperature of 1675°C is recommended, which provides a ~30°C safety margin above the highest intermediate liquidus before endpoint.
- FactSage’s viscosity calculator shows excellent agreement with experiments for sampled compositions containing significant SiO_2 (at least through $\lambda_{O_2} \leq 0.165$). This is a potentially useful tool for calculating viscosities of regolith simulants more generally.

Acknowledgments

- This work was supported by a Lunar Surface Technology Research grant (Award No. 80NSSC24K0129) from NASA's Space Technology Research Grants Program
- The authors would like to acknowledge Kim Scott and Michael Sanders at Colorado School of Mines for assistance with interpretation of DSC data
- Acknowledgments to Sander Bouchard, Halle Kirsten, Yan Ostanin, Lusile Brusoe, Matthew Sato, Julia Esakoff, and Kyla Edison for contributions to the broader MAGMA project activities

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QUESTIONS?

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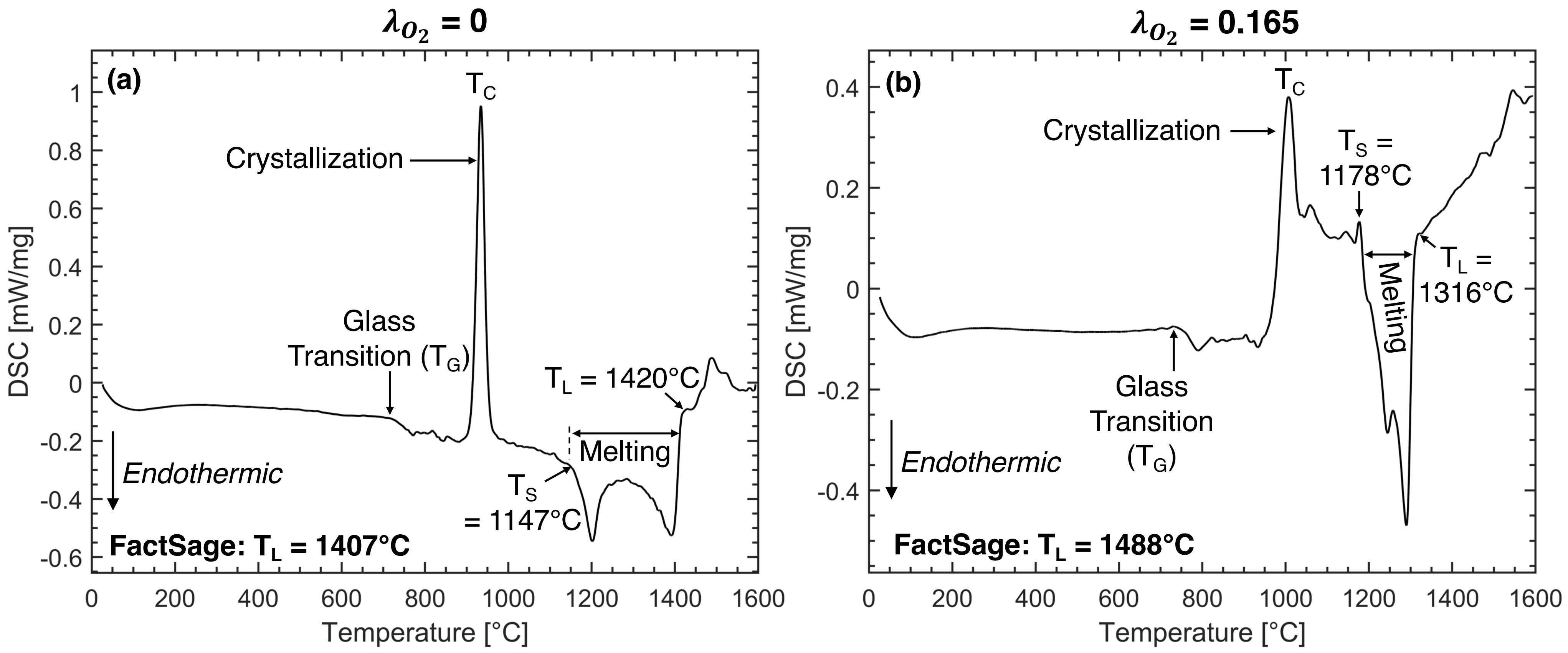
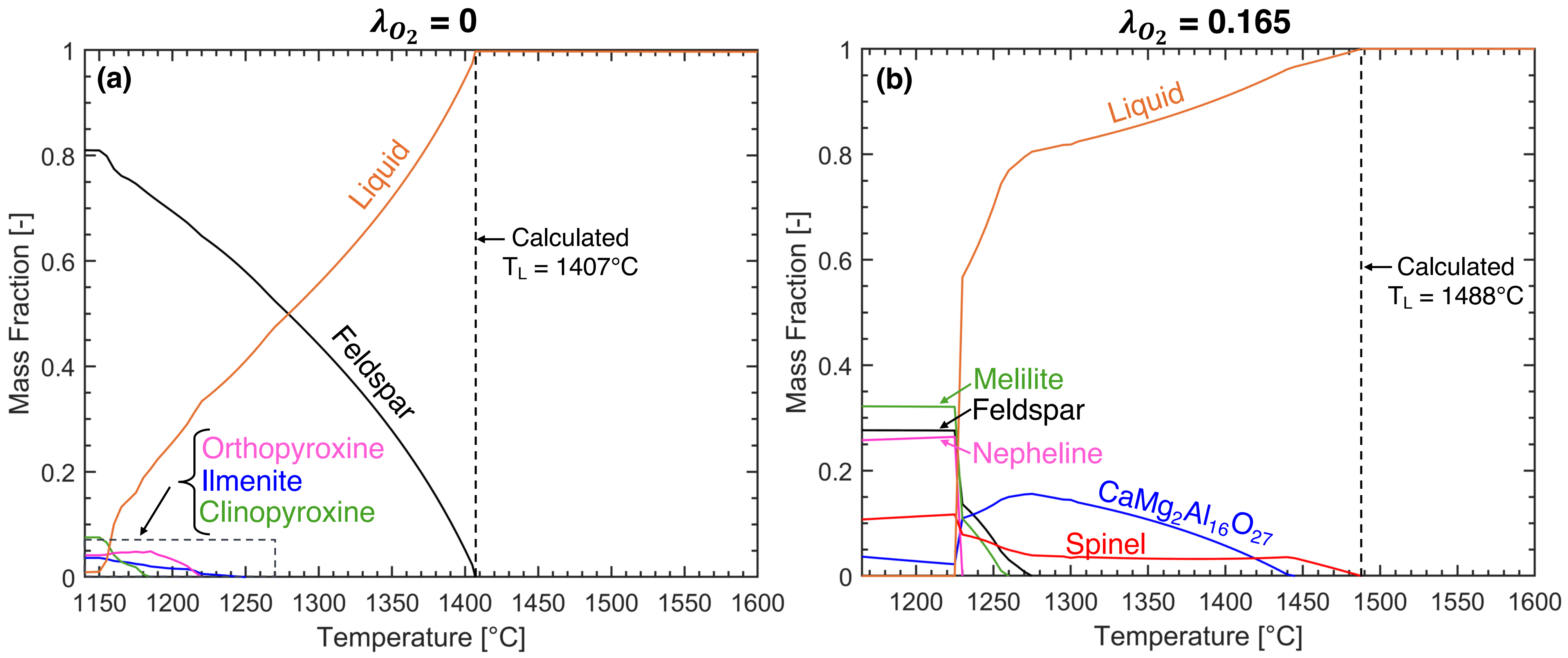
DSC Curves



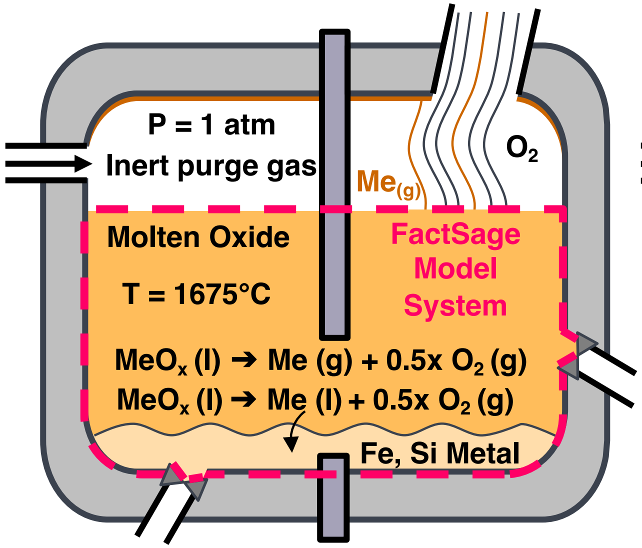
λ_{O_2} = 0
(a)
T_C
Crystallization
Glass Transition (T_G)
T_L = 1420°C
Melting
T_S = 1147°C
Endothermic
FactSage: T_L = 1407°C
DSC [mW/mg]
Temperature [°C]
λ_{O_2} = 0.165
(b)
T_C
Crystallization
T_S = 1178°C
Melting
T_L = 1316°C
Glass Transition (T_G)
Endothermic
FactSage: T_L = 1488°C
DSC [mW/mg]
Temperature [°C]

Single-Axis Diagrams

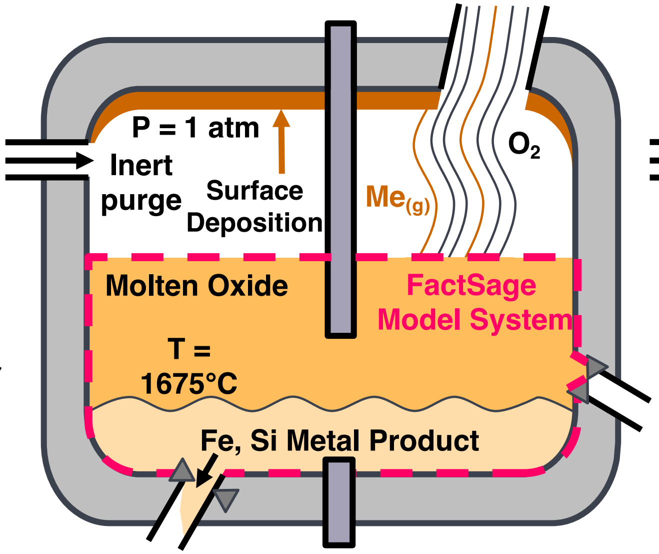


Editable Reactor Schematics

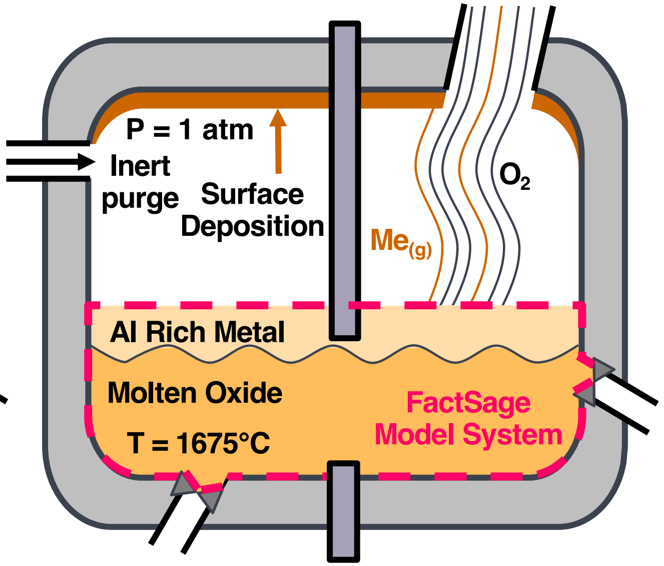
λ_{O_2} << 0.30: Early-Stage Electrolysis (Fe, Si Reduction)



λ_{O_2} = 0.30: Extraction Event 1 (Ferrosilicon Product)



0.30 < λ_{O_2} < 0.37: Late-Stage Electrolysis (Al Reduction)



λ_{O_2} = 0.37 Extraction Event 2 (Aluminum Product)