

How This Works: A Non-Coder's Guide

Cu-Ceramic Thermodynamic Screening Tool

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1 What We Built

An **interactive thermodynamic screening tool** that helps answer: “Which ceramic might best capture copper from molten steel?”

1.1 The Files

File	What it does
<code>cu_ceramic_thermodynamics.py</code>	Main interactive notebook (Marimo) — the one you share
<code>cu_ceramic_affinity.py</code>	Standalone script that generates the Ellingham diagram PNG
<code>pycalphad_cu_fe_example.py</code>	Demo showing how pyCALPHAD library works
<code>ellingham_diagram.png</code>	Static image of oxide stability comparison
<code>cu_fe_gibbs_energy.png</code>	Gibbs energy curves for Cu-Fe system

2 The Thermodynamics Explained

2.1 Gibbs Free Energy (ΔG)

This is the “will it react?” number:

- $\Delta G < 0 \rightarrow$ Reaction happens spontaneously (favorable)
- $\Delta G > 0 \rightarrow$ Reaction won’t happen on its own (unfavorable)

2.2 How We Calculate It

For oxide formation, we use a simple linear approximation:

$$\Delta G_f^\circ = A + B \times T \quad (1)$$

Where:

- A = enthalpy part (kJ/mol) — roughly the “heat” of formation
- B = entropy part (kJ/mol·K) — how “disordered” things get
- T = temperature in Kelvin

2.2.1 Example: Cu_2O

The parameters for Cu_2O are: $A = -170$ kJ/mol, $B = 0.075$ kJ/mol·K
At 1873 K (1600°C):

$$\begin{aligned} \Delta G_f^\circ &= -170 + 0.075 \times 1873 \\ &= -170 + 140.5 \\ &= -29.5 \text{ kJ/mol} \end{aligned} \quad (2)$$

2.3 The Ellingham Diagram

To compare different oxides fairly, we normalize everything to “per mole of O₂”:

Oxide	Reaction	O ₂ in rxn	Divide ΔG _f by
Cu ₂ O	2Cu + $\frac{1}{2}$ O ₂ → Cu ₂ O	0.5 mol	0.5
MgO	Mg + $\frac{1}{2}$ O ₂ → MgO	0.5 mol	0.5
Al ₂ O ₃	2Al + $\frac{3}{2}$ O ₂ → Al ₂ O ₃	1.5 mol	1.5
SiO ₂	Si + O ₂ → SiO ₂	1.0 mol	1.0

Key insight: Lower on the diagram = more stable oxide.

2.4 What the Diagram Tells Us

Cu₂O is at the **TOP** (least stable). This means:

- Cu **cannot steal oxygen** from Al₂O₃, MgO, SiO₂, or TiO₂
- The reaction Cu + Al₂O₃ → Cu₂O + Al will **NOT** happen
- We need a *different mechanism* to capture Cu

2.5 The Actual Mechanisms

Since Cu can't reduce the oxides, how does Al₂O₃ capture Cu? (It did in last year's experiments)

1. **Solid Solution** — Cu atoms dissolve into the ceramic crystal at high T
2. **Spinel Formation** — CuAl₂O₄ forms (requires Cu to oxidize first)
3. **Surface Adsorption** — Cu sticks to particle surfaces
4. **Capillary Action** — Molten Cu wets and penetrates porous ceramics

2.6 Sulfide Exchange (The Alternative)

Dr. Zhang showed this reaction works:



Why? Because Cu₂S is more stable than FeS (ΔG < 0 for this reaction).

3 How the Code is Structured

3.1 The Marimo Notebook Format

Marimo notebooks are Python files with special structure:

```
import marimo
app = marimo.App()

@app.cell           # This decorator marks a "cell"
def _():
    # Code goes here
```

```

    return variables_to_share

@app.cell
def _(variables_from_above):
    # This cell can use those variables
    return more_variables

```

3.2 Key Parts of Our Notebook

3.2.1 1. Data Definition

The oxide data is stored in a Python dictionary:

```

oxide_data = {
    'Cu2O': (-170, 0.075, 0.5, '#0077BB', '--', '2Cu + 1/2O2 -> Cu2O'),
    #          A        B      O2_factor   color   linestyle   reaction
}

```

3.2.2 2. Calculation Functions

```

def calc_dGf_per_O2(name, T_K):
    A, B, O2_factor, *_ = oxide_data[name]
    return (A + B * T_K) / O2_factor

```

3.2.3 3. Interactive Controls

```

temp_slider = mo.ui.slider(start=1000, stop=1700, value=1600)
oxide_selector = mo.ui.multiselect(options=[...], value=[...])

```

4 How to Make Changes

4.1 Change the Temperature Range

Find this line and edit the numbers:

```
temp_slider = mo.ui.slider(start=1000, stop=1700, ...)
```

4.2 Add a New Oxide

Add an entry to `oxide_data`:

```
'NewOxide': (A_value, B_value, O2_factor, '#HexColor', '--', 'Reaction'),
```

Where:

- Look up A and B values from thermodynamic tables (NIST-JANAF, Barin)
- O_2 _factor = moles of O_2 in the formation reaction
- Color = hex code (colorblind-friendly: #0077BB, #EE7733, #009988)

4.3 Change Label Positions

Find the `_min_spacing` variable in the plot cell:

```
_min_spacing = 45 # Increase for more space between labels
```

5 Limitations

Warning: This tool uses **simplified approximations**. It is a screening tool, not rigorous CALPHAD.

Limitation	Why it matters
No activity coefficients	Real solutions aren't ideal
No phase diagrams	Can't find two-phase regions
No Cu solubility in oxides	This is the real mechanism!
No kinetics	Doesn't tell you how fast
Linear ΔG approximation	Real curves have more terms

For real CALPHAD calculations, you need Thermo-Calc with proper databases.

6 Next Steps: Thermo-Calc

6.1 What Thermo-Calc Can Do That This Can't

1. **Proper phase diagrams** — Cu-Fe-O, Cu-Al-O ternary sections
2. **Cu solubility** — How much Cu dissolves in Al_2O_3 at 1600°C?
3. **Activity coefficients** — Real solution behavior
4. **Equilibrium calculations** — What phases are stable?

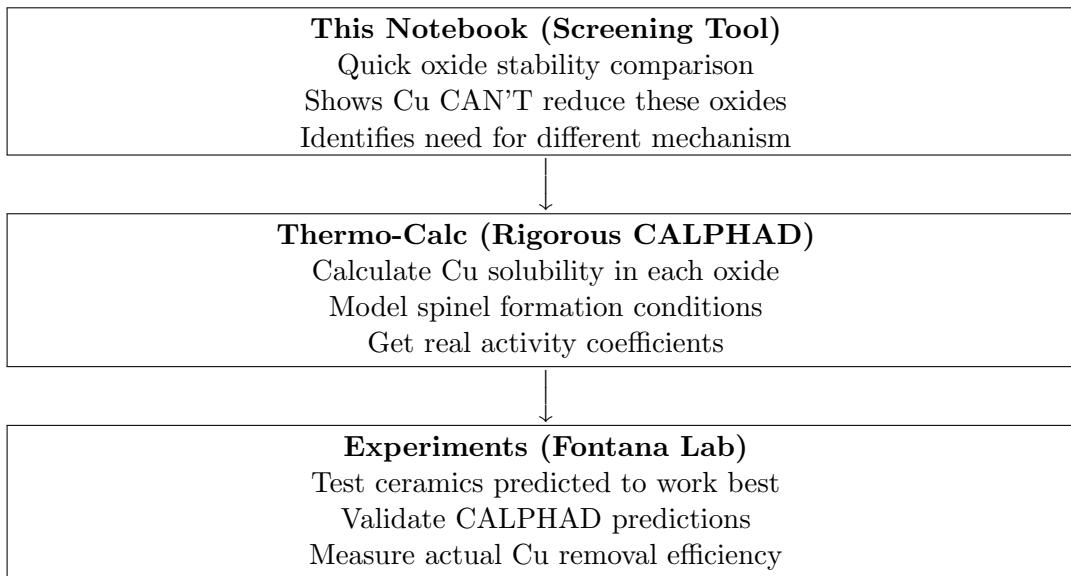
6.2 Databases You Need

Database	Contents	Use for
TCFE	Steel thermodynamics	Cu in liquid Fe
TCOX	Oxide systems	Cu-Al-O, Cu-Mg-O
SSUB	Pure substances	Reference data

6.3 Calculations to Run in Thermo-Calc

1. **Cu-Fe binary phase diagram** — Understand Cu miscibility in Fe
2. **Cu activity in liquid Fe** — At 1600°C, how “active” is 0.3% Cu?
3. **Cu-Al-O isothermal section at 1600°C** — What phases form?
4. **Property diagram: Cu solubility in Al_2O_3 vs T** — The key data we need

7 Workflow Summary



8 Reference: Thermodynamic Data

8.1 Oxide Parameters Used

Oxide	A (kJ/mol)	B (kJ/mol·K)	O ₂ factor	Source
Cu ₂ O	-170	0.075	0.5	NIST-JANAF
CuO	-155	0.085	0.5	NIST-JANAF
FeO	-264	0.065	0.5	NIST-JANAF
Al ₂ O ₃	-1676	0.32	1.5	NIST-JANAF
MgO	-601	0.11	0.5	NIST-JANAF
SiO ₂	-910	0.18	1.0	NIST-JANAF
TiO ₂	-944	0.18	1.0	NIST-JANAF

Table 1: Gibbs energy parameters for oxide formation ($\Delta G_f^\circ = A + BT$). Values are approximations.

8.2 Sulfide Parameters

Sulfide	ΔG_f approximation	Source
FeS	$-150 + 0.027T$	Literature estimate
Cu ₂ S	$-180 + 0.032T$	Literature estimate

Table 2: Gibbs energy parameters for sulfide formation.

9 Links

- **GitHub Repository:** <https://github.com/dimascad/honda-calphad>
- **Interactive Notebook:** Open via Marimo from GitHub link
- **Marimo Documentation:** <https://docs.marimo.io>