# How This Works: A Non-Coder's Guide

Cu-Ceramic Thermodynamic Screening Tool

Anthony DiMascio

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## Contents

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

# 2 The Thermodynamics Explained

## 2.1 Gibbs Free Energy ($\Delta G$)

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:

$$\boxed{\Delta G_f^\circ = A + B \times T} \tag{1}$$

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):

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

### 2.3 The Ellingham Diagram

To compare different oxides fairly, we normalize everything to "per mole of $O_2$":

| Oxide | Reaction | $O_2$ in rxn | Divide $\Delta G_f$ by |
|---|---|---|---|
| $Cu_2O$ | $2Cu + \frac{1}{2}O_2 \rightarrow Cu_2O$ | 0.5 mol | 0.5 |
| MgO | $Mg + \frac{1}{2}O_2 \rightarrow MgO$ | 0.5 mol | 0.5 |
| $Al_2O_3$ | $2Al + \frac{3}{2}O_2 \rightarrow Al_2O_3$ | 1.5 mol | 1.5 |
| $SiO_2$ | $Si + O_2 \rightarrow SiO_2$ | 1.0 mol | 1.0 |

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

### 2.4 What the Diagram Tells Us

$Cu_2O$ is at the **TOP** (least stable). This means:

- Cu **cannot steal oxygen** from $Al_2O_3$, MgO, $SiO_2$, or $TiO_2$
- The reaction $Cu + Al_2O_3 \rightarrow Cu_2O + Al$ 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 $Al_2O_3$ 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** — $CuAl_2O_4$ 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:

$$2Cu + FeS \rightarrow Cu_2S + Fe \tag{3}$$

Why? Because $Cu_2S$ is more stable than FeS ($\Delta G < 0$ 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)
- O2_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 $\Delta G$ 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?

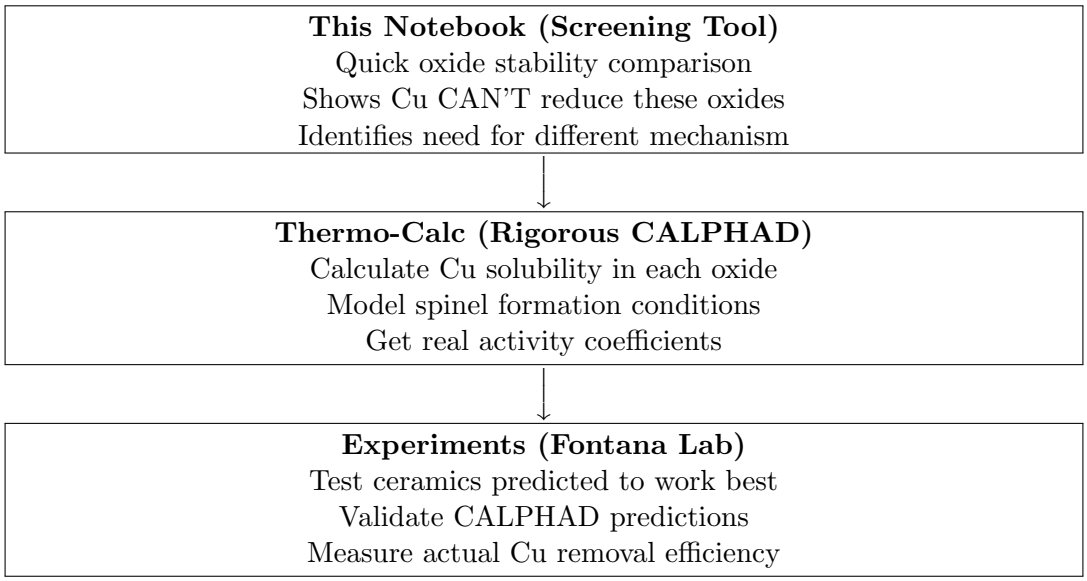
### 6.2 Databases You Need

| 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 |
|---|---|---|---|---|
| $Cu_2O$ | −170 | 0.075 | 0.5 | NIST-JANAF |
| CuO | −155 | 0.085 | 0.5 | NIST-JANAF |
| FeO | −264 | 0.065 | 0.5 | NIST-JANAF |
| $Al_2O_3$ | −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 | $\Delta G_f$ approximation | Source |
|---|---|---|
| FeS | $-150 + 0.027T$ | Literature estimate |
| $Cu_2S$ | $-180 + 0.032T$ | Literature estimate |

Table 2: Gibbs energy parameters for sulfide formation.

# 9 Links

- **GitHub Repository:** https://github.com/dimascad/honda-calphad
- **Interactive Notebook:** https://molab.marimo.io/notebooks/nb_ZnGGazDX6TcpFZz6w9yaw3/app
- **Marimo Documentation:** https://docs.marimo.io