Thermodynamic Calculations with a Low Threshold: Excel Worksheets, 3D Phase Diagrams and Other Educational Tools

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Abstract

Thermodynamic calculations and phase diagrams are powerful tools for the understanding and optimization of metallurgical high-temperature processes. With its recent developments, *InsPyro* aims to make them more accessible, more versatile, and - if still possible - more fun.

1. With the development of a customized interface, *InsPyro* wants to make the use of thermodynamic calculations easier and more robust. It was decided to work with an Excel interface as this is well-known and widespread for data processing.

   The example worked out in this presentation is the case of a process model integrated in charge calculation for a lead recycling furnace. From the weights of scrap, fluxes, reductants and any other materials added, the tool can estimate:

   - The amount and composition of the lead alloy that will be produced, and similar for slag and matte if present
   - The amount of heat required to melt the material (or produced from reactions)
   - The excess amount of reductants
   - The amount of SO_2 in the gas phase

   This provides easy feedback on the charge before it is loaded into the furnace. With a simple click of a button, the effect of adjustments to correct imbalances can be seen immediately.

2. As phase diagrams give valuable information on the relations between different phases, they bring a deeper understanding of microstructure formation and material properties. However, to extract this information out of a phase diagram is not always easy. In our experience, the representations of binary systems are well understood, but are also a discussion tool where people want to write on, compare microstructures with, and so on. Therefore we developed a whiteboard phase diagram, which allows you to do this without any hi-tech: just a marker, eraser, magnets...
3. Discussion and insight becomes more difficult if a process can no longer be explained by a simple binary approximation. Multicomponent systems are usually represented by e.g. liquidus projections, isothermal sections, and vertical sections. To understand how a multicomponent system behaves, spatial insight is required. Representing the phase diagram in three dimensions helps to visualize the phase relations. InsPyro realized a physical 3D prototype using rapid manufacturing techniques. In this workshop we want to present this and want to discuss with the audience how these tools can be optimized.

These developments are part of our continued efforts to make thermodynamics more accessible in metallurgy, for a broad audience from engineers at SME's, over production staff in large companies, to R&D departments and university students.