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Interactive visualization of pyrometallurgical phase diagrams

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Introduction: what are phase diagrams used for?

- Ores contain valuables & gangue material
- Pyrometallurgy = high temperature processing (1000 – 1800℃)
- Gangue, e.g. SiO_2, Al_2O_3, etc. form ”slag” = mixture of **molten oxides**
- Separation ~ density difference between metal & slag

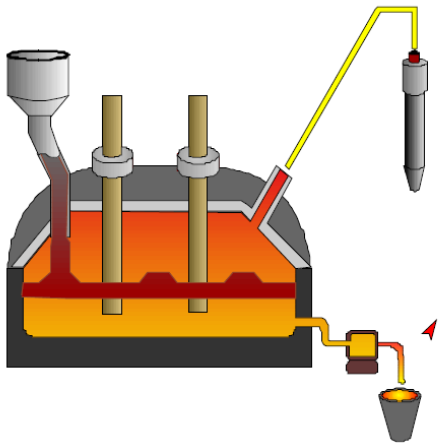
INPUT

Ore (Chromite)

Reductants
Coke
Coal
Char

Flux (Silica)

Water



OUTPUT

Ferrochrome

Slag

Slimes

Gases

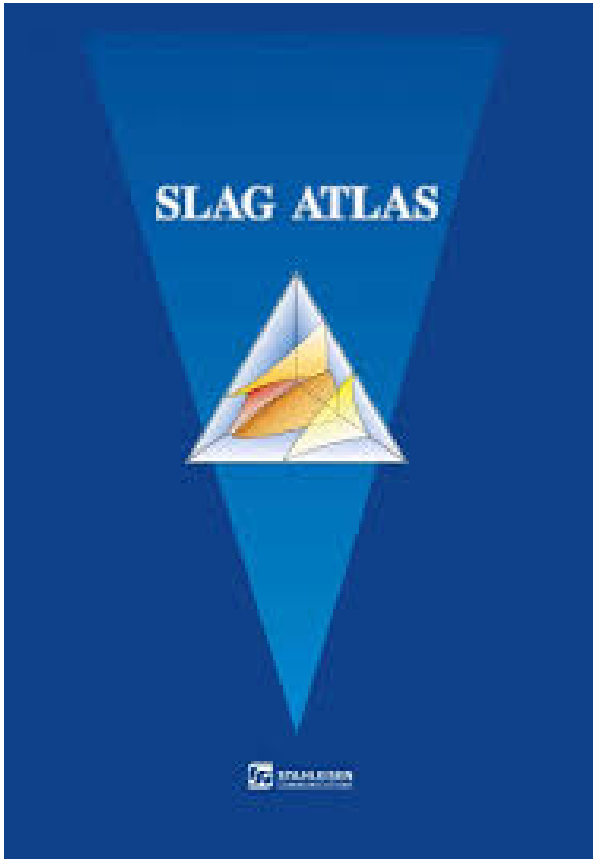
SO_2 NO_2 CO_2

TSP Water

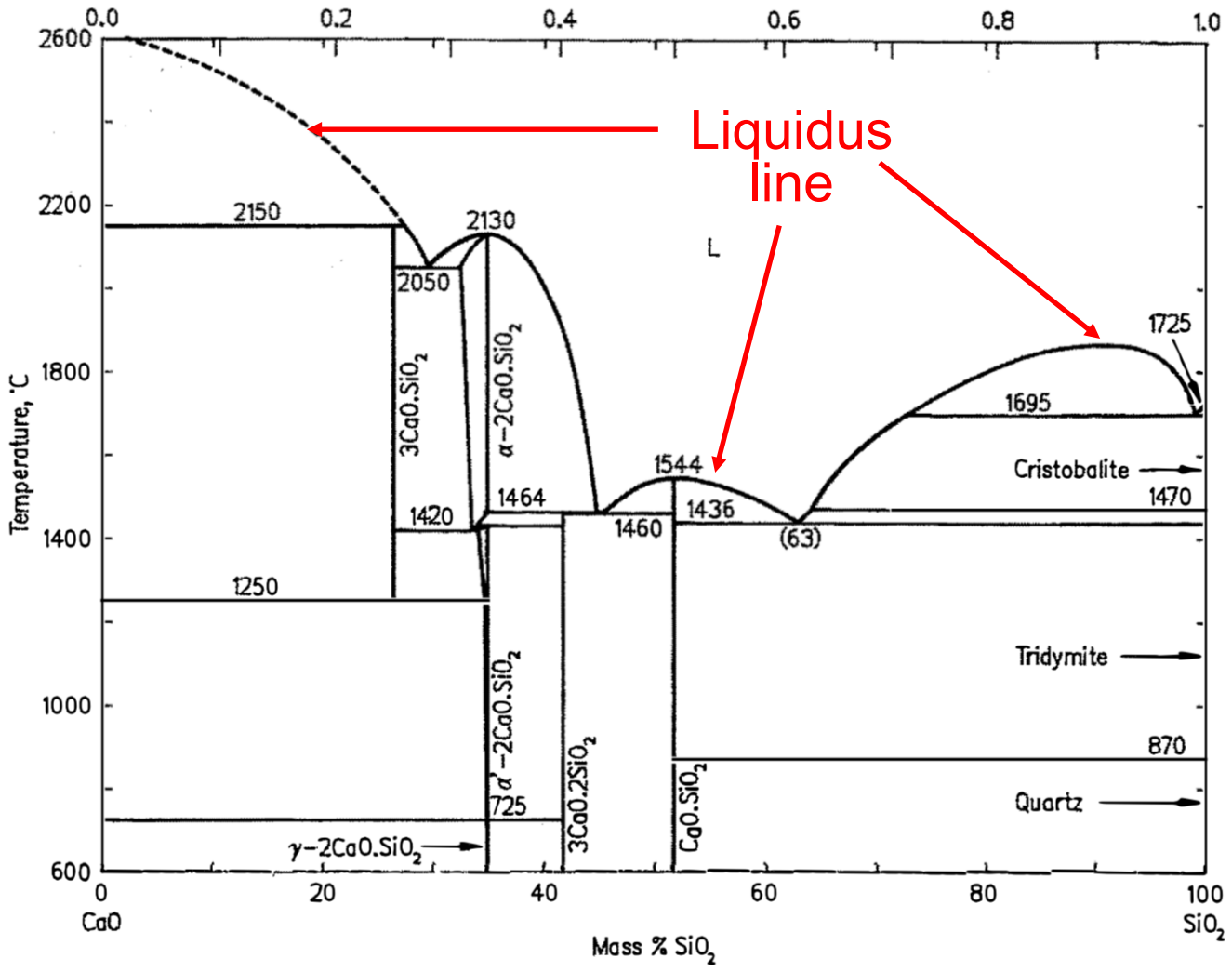
Naiker, 2006

The “Bible” of phase diagrams: Slag Atlas

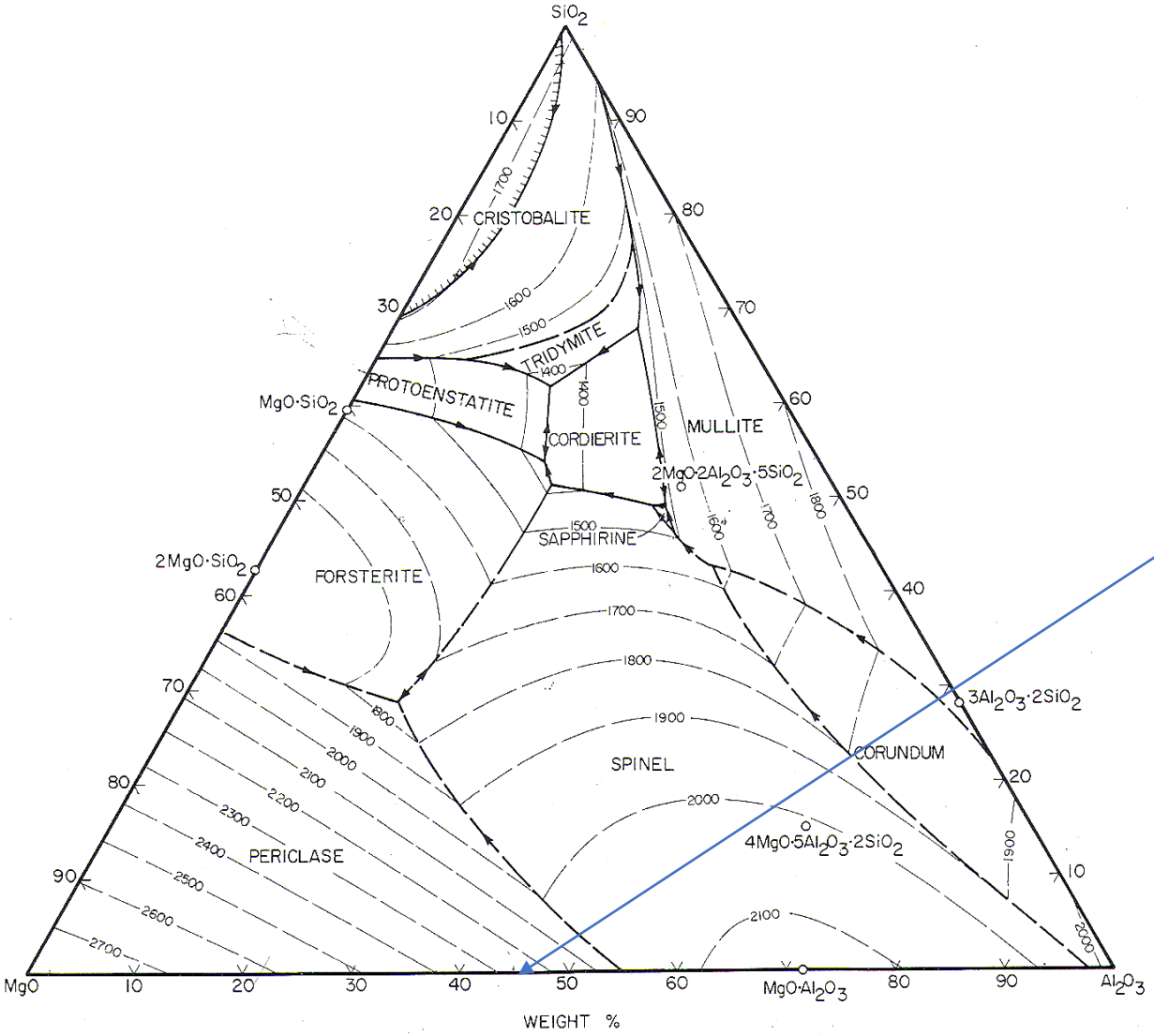
- Collection of oxide slag data
- Based on 1000s of papers
- Published in 1995 (23 years ago)
- References date back to as early as 1900

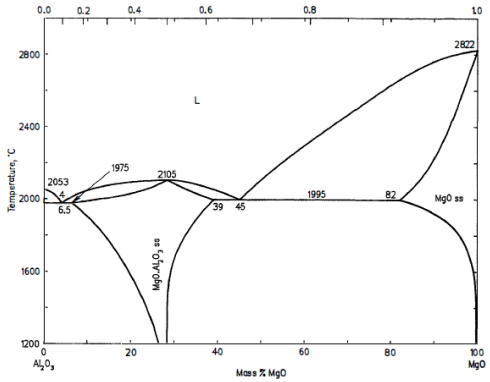


Lower the melting point ("liquidus") of gangue: use fluxes

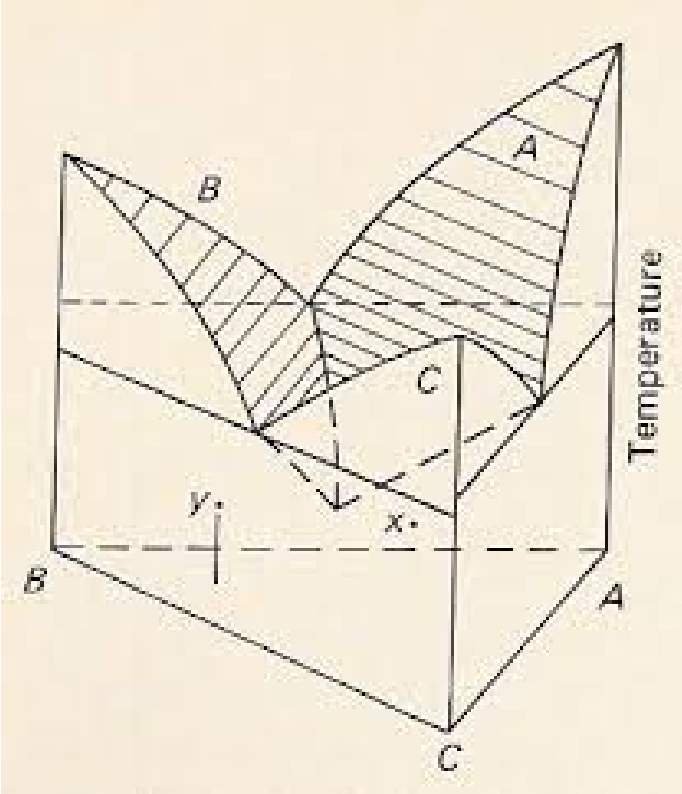


But ores (and hence slags) contain more than 2 components…

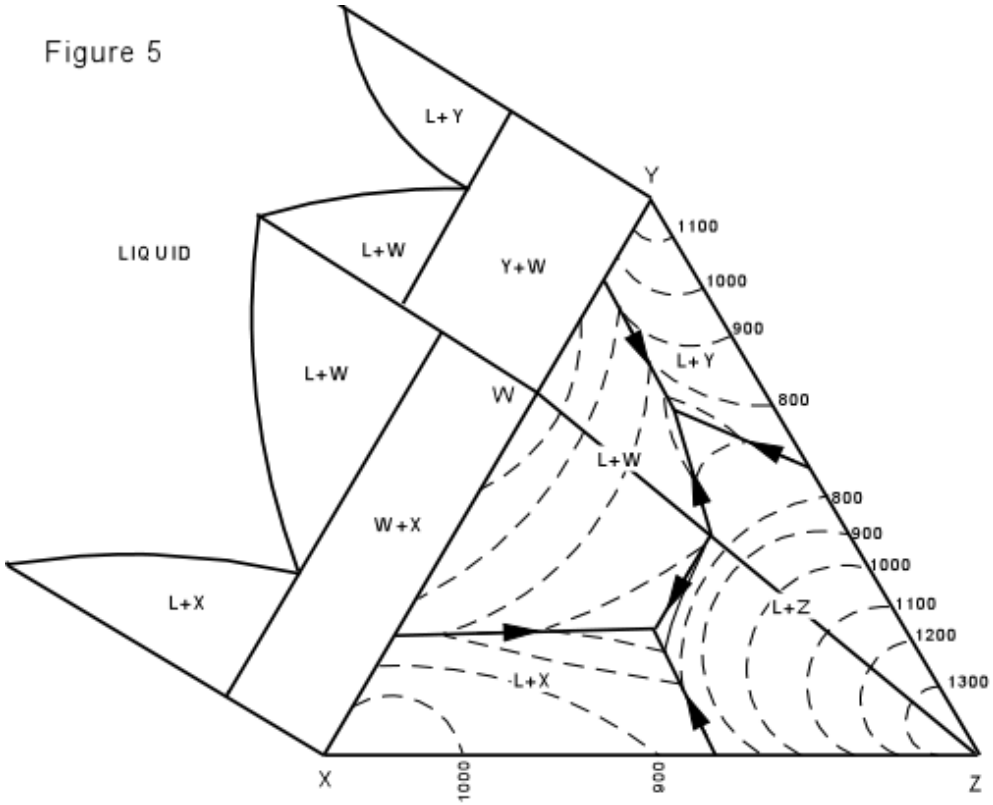




Ternary diagrams are projected into 2D contour plots



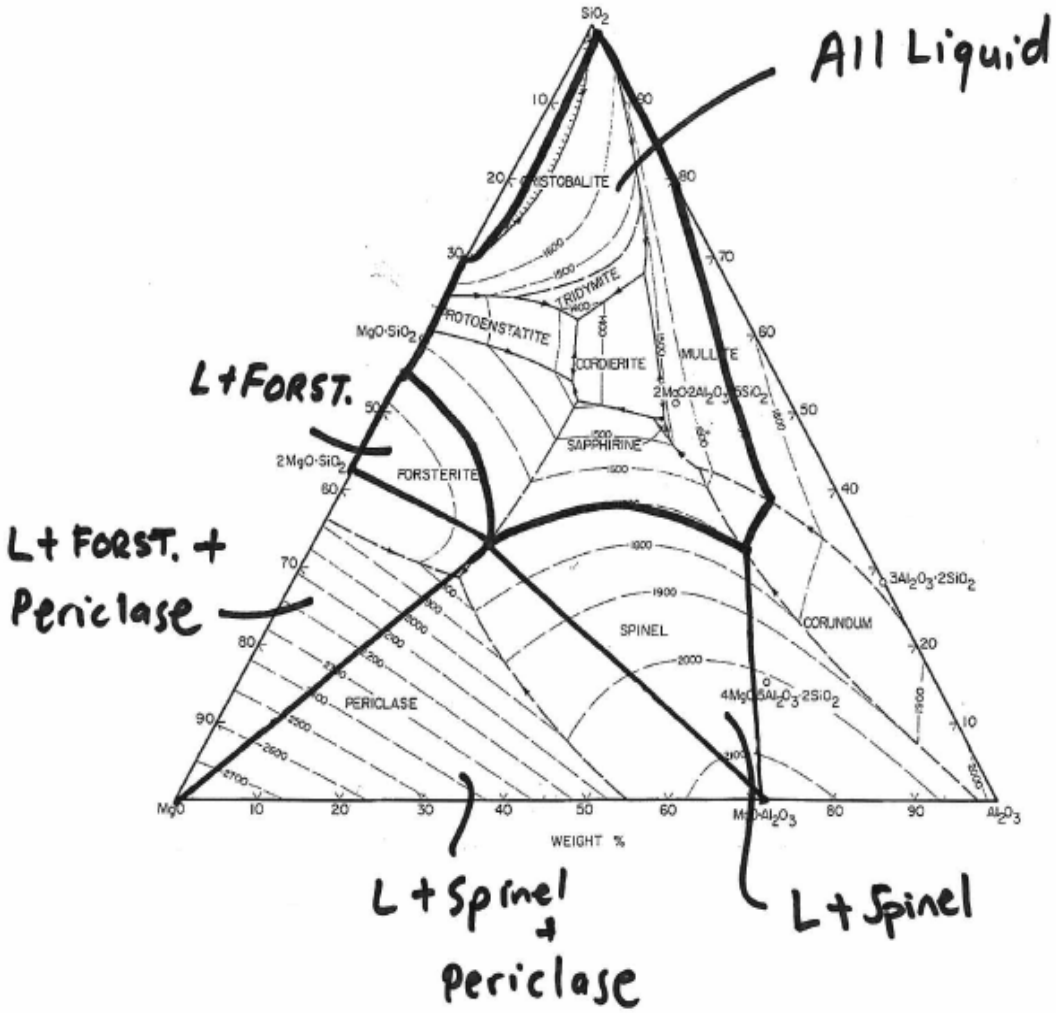
http://plate-tectonic.narod.ru/ptrphasemore2componphotoalbum.html



https://www.tulane.edu/~sanelson/eens212/ternaryphdiag.htm

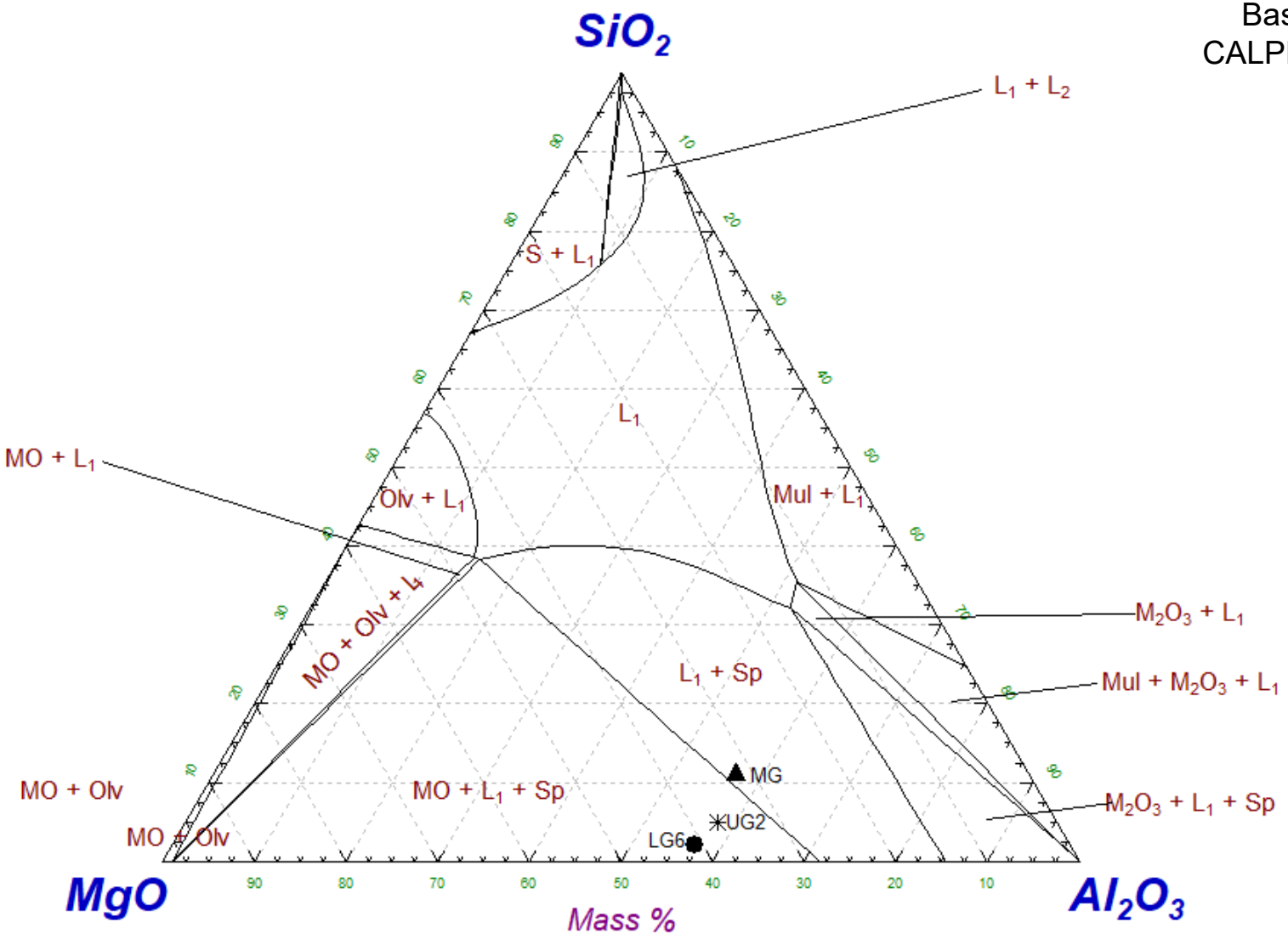
Liquidus surface: areas of composition where slag is fully molten

- By hand:



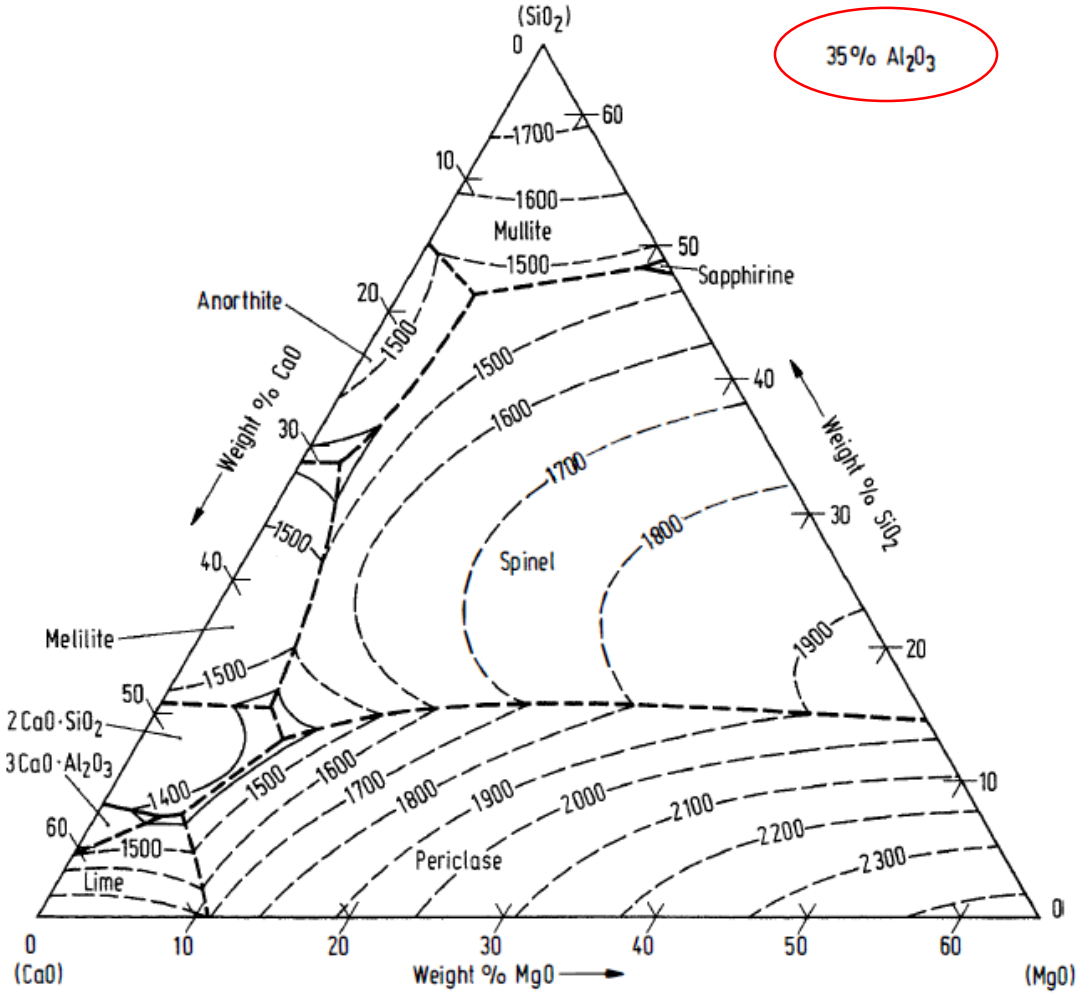
More modern tools, e.g. FactSage™

Based on the CALPHAD method



It gets even more complicated: Quad-ternary diagram

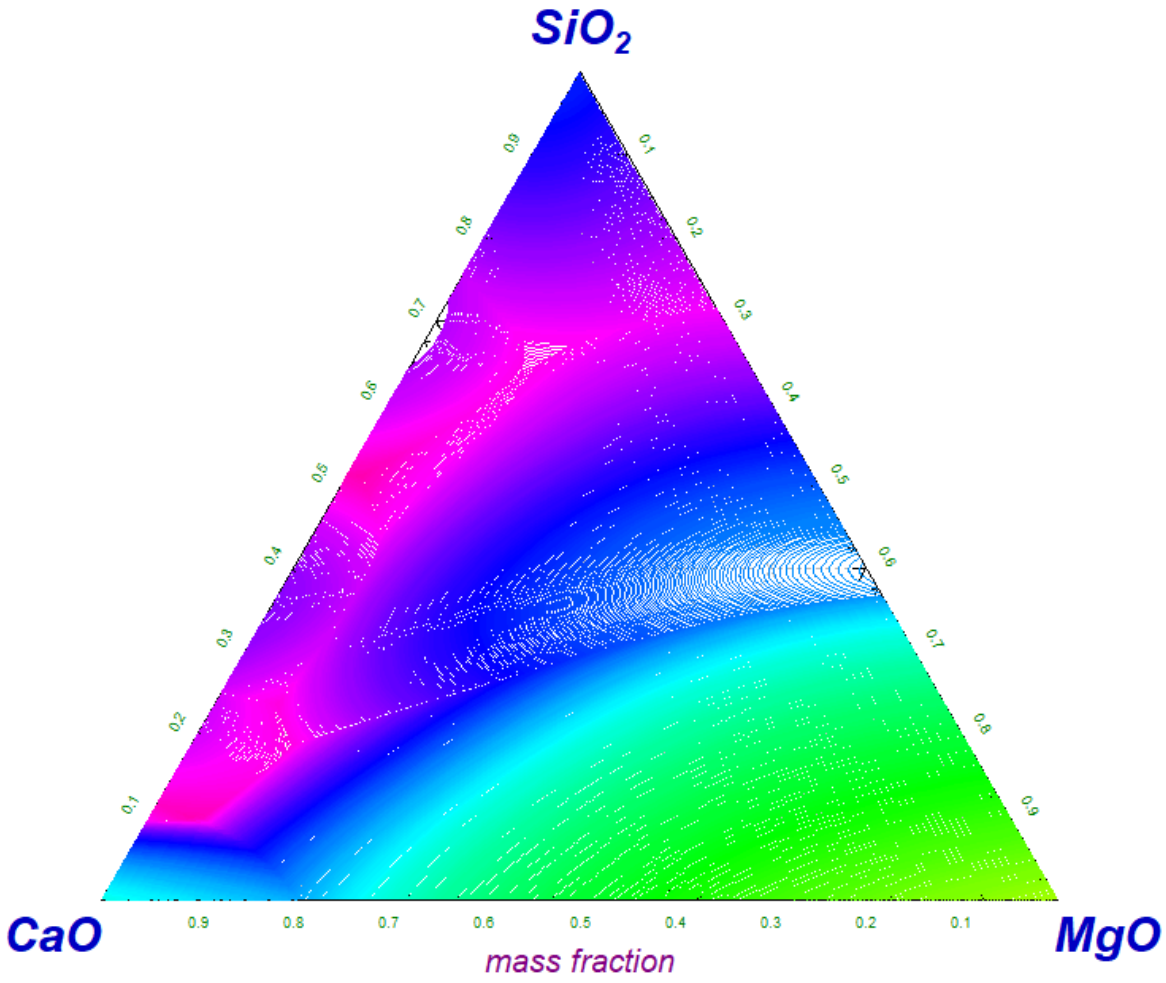
- 4 components system: a slice at constant composition …

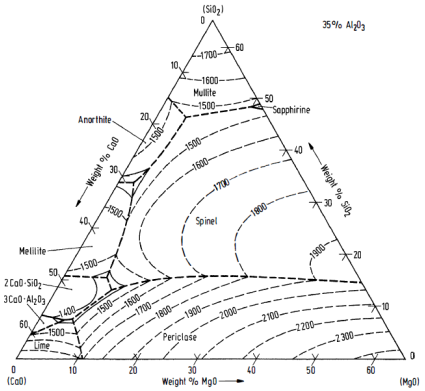


Possible to generate data sets and visualize data a bit better

- Modern tools allow for generating large data sets through digital experiments, e.g. FactSage™
- Classical metallurgists meet high performance computing & data science experts…
- Visualization easily achieved using open-source tools:
  - Python (for a bit of data cleanup, interpolation)
  - ParaView for visualization

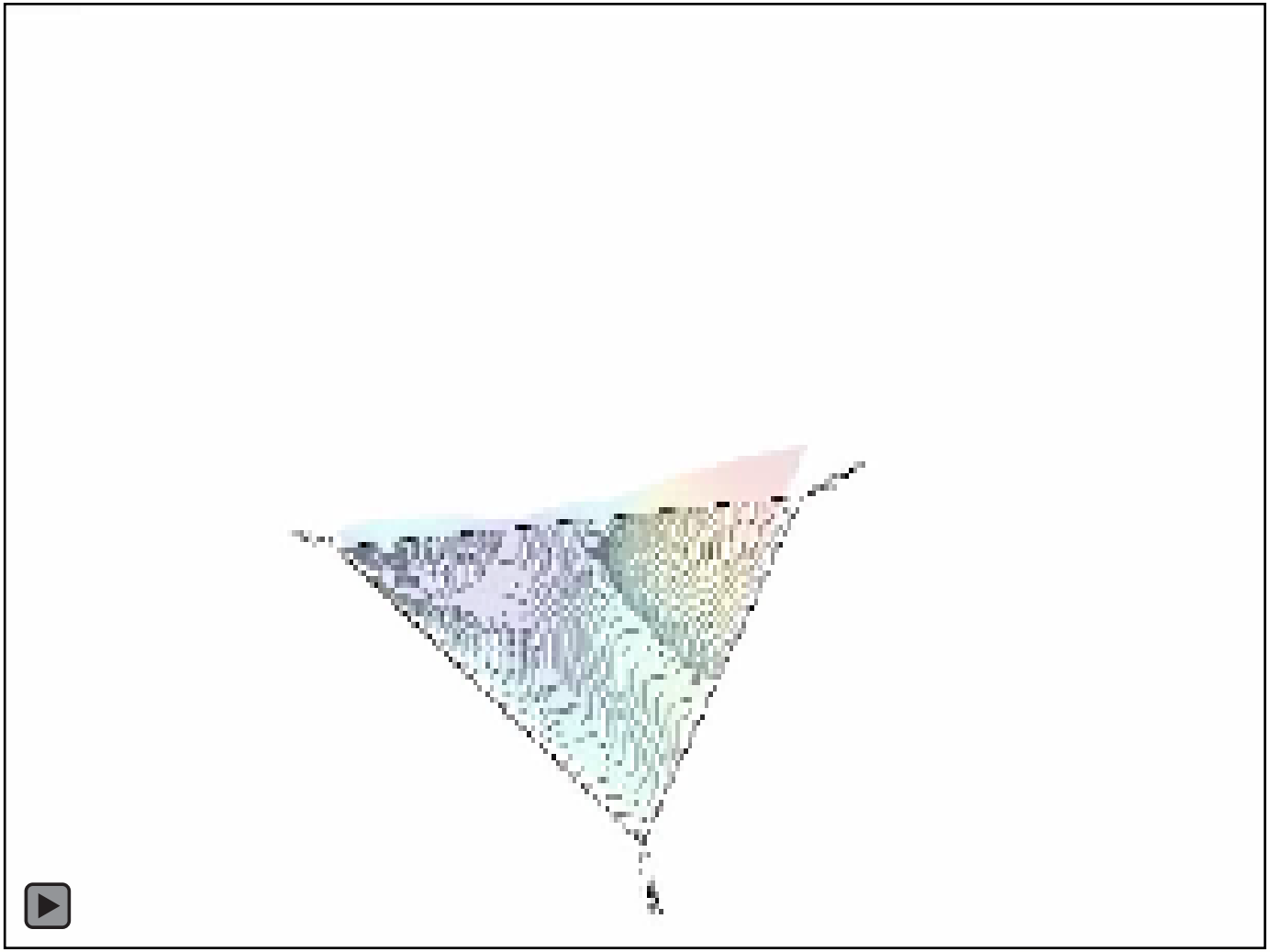
Quad-ternary diagram (FactSage) – high resolution (35% Al_2O_3)





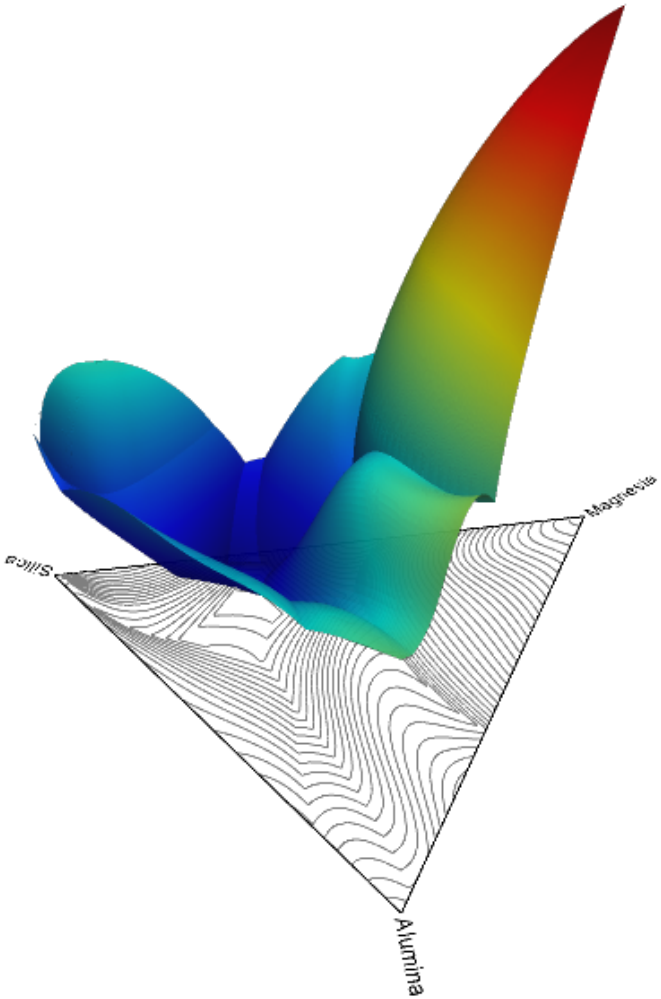
Visualization of phase diagrams can be useful

- Animation might help a bit, especially if you are new to this…



Note: In PDF version of this file you will need flash player installed to play this video

3D representation of liquidus surface: MgO-Al_2O_3-SiO_2

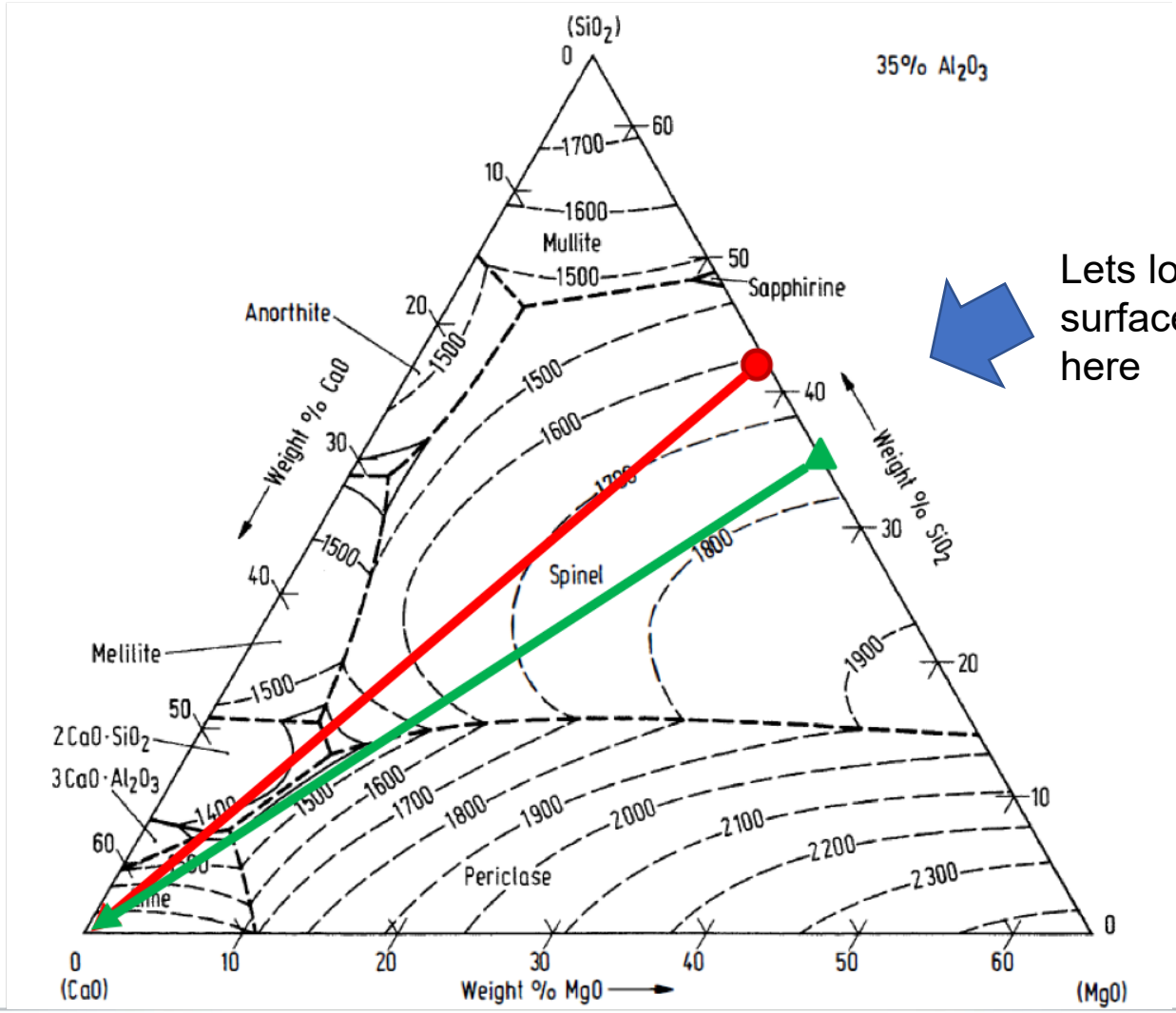


A more practical way at designing slags

- Chromite ores are fluxed with SiO_2 and CaO
- SiO_2 drops the melting point, but makes slag viscous
- CaO drops the viscosity, but can increase melting point
- Balance between the two driven by the original composition of the ore
- Need to look at the quad-ternary (4 component) phase diagram
- How sensitive is the slag melting point to adding CaO?

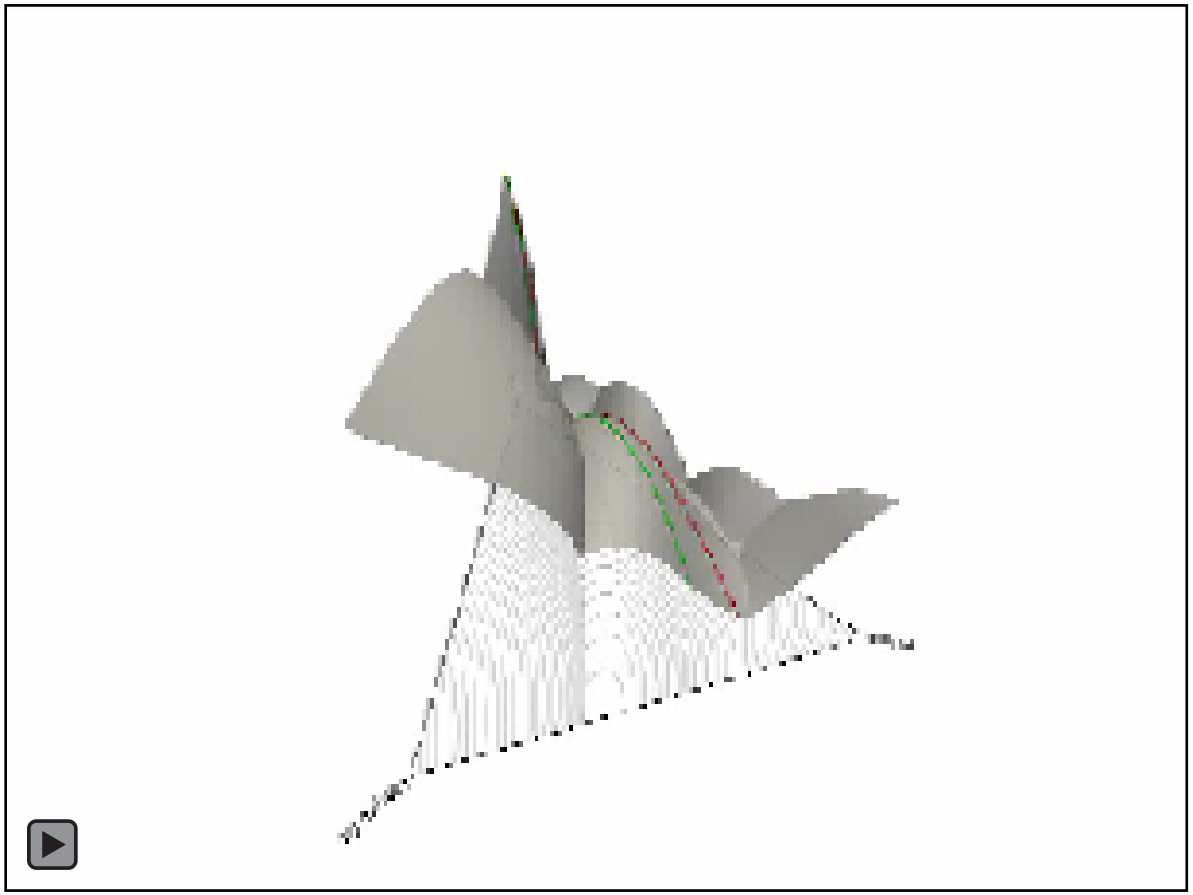
Adding CaO to MgO-Al2O3-SiO2 slags: effect on melting point

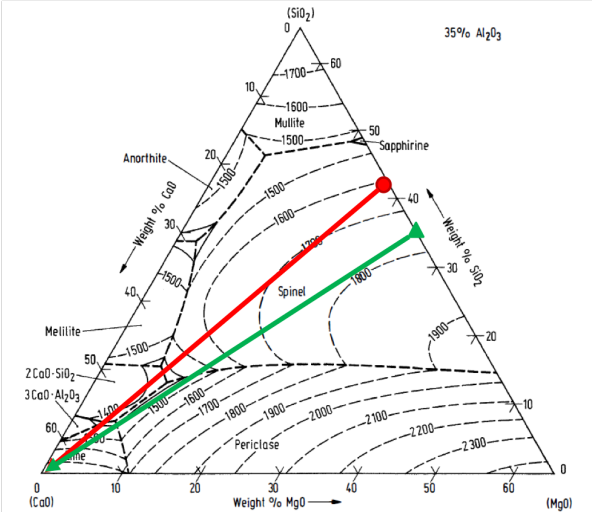
- Classical view:



Lets look at the surface in 3D from here

The view in 3D





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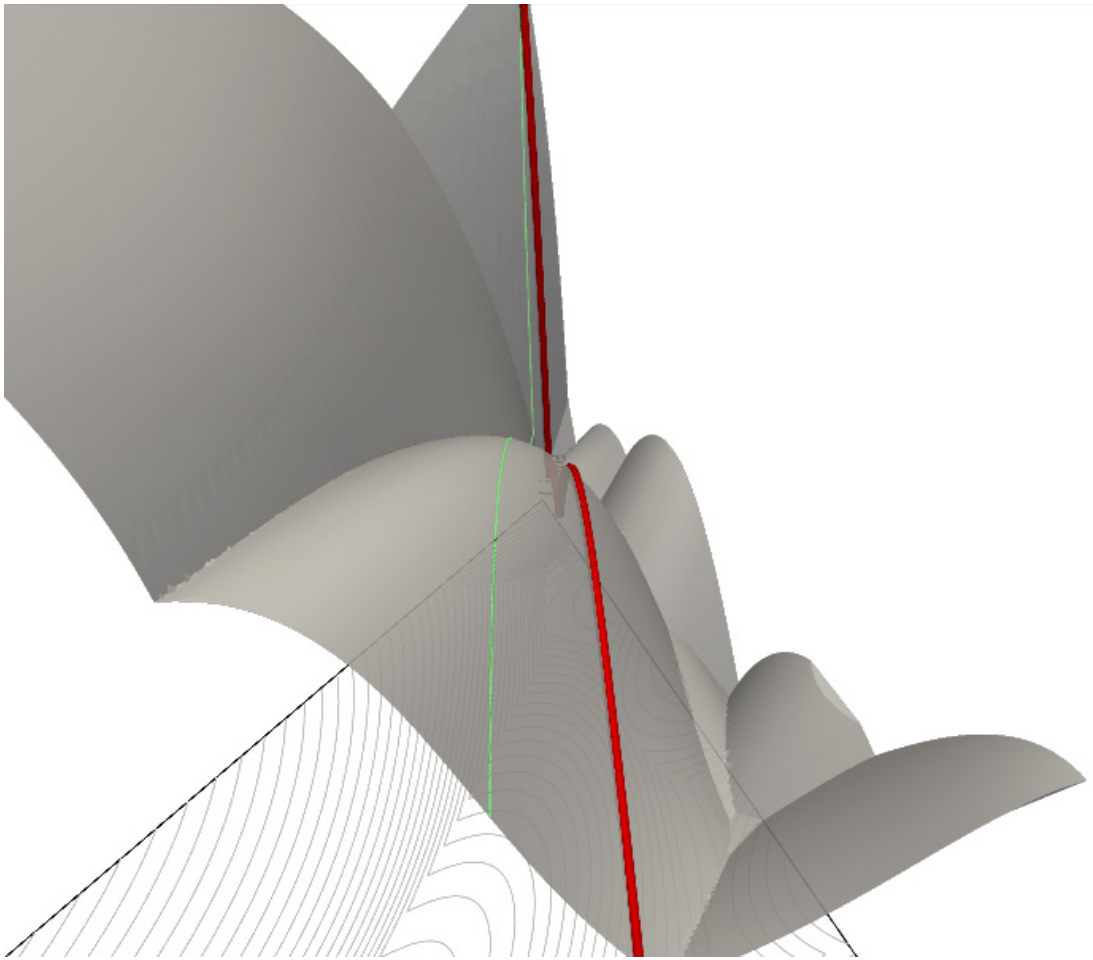
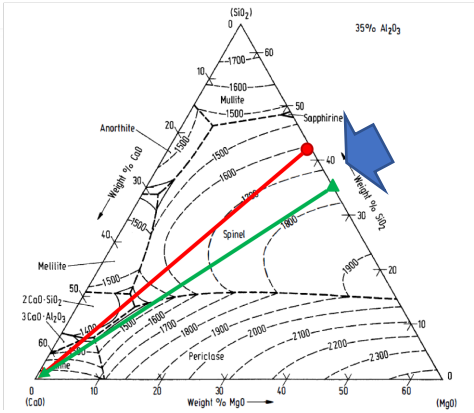
”A higher liquidus is more forgiving”

- Sensitivity of two slags to CaO addition





Final thoughts

- This is just one way of looking at phase diagrams
  - For the novice: get a bit more insight in 3D
  - For the expert: evaluate data for errors

- Idea is to create a generic way of looking at multiple forms of data, good for teaching / learning

- Many tools are open-source and well established

- Need to think outside of your classical training

- Adopt a data scientist?!

ACKNOWLEDGEMENTS