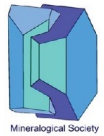
Day 5, Part 1
THERMOCALC, Perple_X and Theriak-Domino*: What are the key differences?

* Other codes are available!

PHASE EQUILIBRIUM MODELLING: APPROACHES AND PITFALLS



Which program should I use to model my [*insert rock type here*]?

Which thermodynamic dataset should I use to model my [*insert rock type here*]?

- Do the components considered within the dataset allow a reasonable description of your rock's composition?
- Are there end-members in the dataset that would outline all of the key phases in the rock?
- Are there solution (*a-X*) models for the phases of interest?
- Do the calibrations extend to the range of *P-T* conditions that you are interested in?

Jacob will discuss thermodynamic system complexity in more detail later today

Thermodynamic Data

	THERMOCALC	Perple_X	Theriak-Domino
I want to calculate with the most recent version of the Holland & Powell dataset	✔	✔ (with caution)	✔ (with caution)
I want to calculate with a legacy version of the Holland & Powell dataset	?	✔	✔
I want to calculate with the Berman data	✘	✔	✔
I want to calculate with the supcrt92 data	✘	✔	✔ (undocumented)
I want to calculate with the Stixrude & Lithgow-Bertelloni data	✘	✔	✘
I want a dataset that lets me calculate seismic properties	✘	✔ (with caution)	? (not straightforward)
I want a dataset that lets me calculate fluid speciation	✘	✔ (with caution)	✔ (Theriaq, but it isn't ready)

Thermodynamic Data

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I want to calculate with a legacy version of the Holland & Powell dataset	?	✔	✔
I want to calculate with the Berman data	✘	✔	✔
I want to calculate with the supcrt92 data	✘	✔	✔ (undocumented)
I want to calculate with the Stixrude & Lithgow-Bertelloni data	✘	✔	✘
I want to be completely insulated from choosing which version of a solution model pairs best with end-member data	✔	✘	✔ / ✘
I want to be free to make potentially dubious decisions of pairing old models with new data (and vice versa), and using models calibrated with different datasets	✘	✔	✔ / ✘

Thermodynamic Data

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I want to calculate with the Berman data	✘	✔	✔
I want to calculate with the supcrt92 data	✘	✔	✔ (undocumented)
I want to calculate with the Stixrude & Lithgow-Bertelloni data	✘	✔	✘
I want to code in my own solution models	Tricky, but possible. Inadvisable?	Fairly easy	Fairly easy (apparently)

Calculation Types

	THERMOCALC	Perple_X	Theriak-Domino
I want to calculate a petrogenetic grid	✔	✔ (be advised)	✘
I want to calculate AFM diagrams	✔	✔	✔
I want to calculate phase assemblage diagrams (*P-T*, *T-X* or *P-X*) for a system of known composition	✔	✔	✔
I want to demonstrate dataset uncertainties in my diagrams	✔	✘ *	✘ *
I want the mineral assemblage to be buffered by a fluid of constrained composition	✔	✔	✔ / ✘ (see Doug's talk)
I want to do inverse modeling to calculate *P* & *T* from phase compositions	✔	✘	✔ / ✘ (the Lanari approach)

* But you can use THERMOCALC-derived constraints on uncertainty and apply them, at least semi-quantitatively

Calculation Types

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I want to calculate phase assemblage diagrams (*P-T*, *T-X* or *P-X*) for a system of known composition	✔	✔	✔
I want to demonstrate dataset uncertainties in my diagrams	✔	✘ *	✘ *
I want the mineral assemblage to be buffered by a fluid of constrained composition	✔	✔	✔ / ✘ (see Doug's talk)
I want to do inverse modeling to calculate *P* & *T* from phase compositions	✔	✘	✔ / ✘ (the Lanari approach)
Have other people written 'add-on' or 'helper programs' to streamline workflow or add value to results?	✔	✔	✔

For the Case of Phase Assemblage Diagram Calculations

	THERMOCALC	Perple_X	Theriak-Domino
I want to build this line-by-line, so I really understand the outcome	✔	✘	✘
I don't have the patience for that! I want automation	✘	✔	✔

This deserves more thought:

- Slowly deriving a diagram 'by hand' (line-by-line) can be a **GREAT** thing – it leads to better understanding of the phase equilibria.
- Rapidly deriving a diagram automatically by G minimization can also be a **GREAT** thing – it allows us to explore how sensitive results are to, for example, small changes in rock composition or changes in activity-composition models.

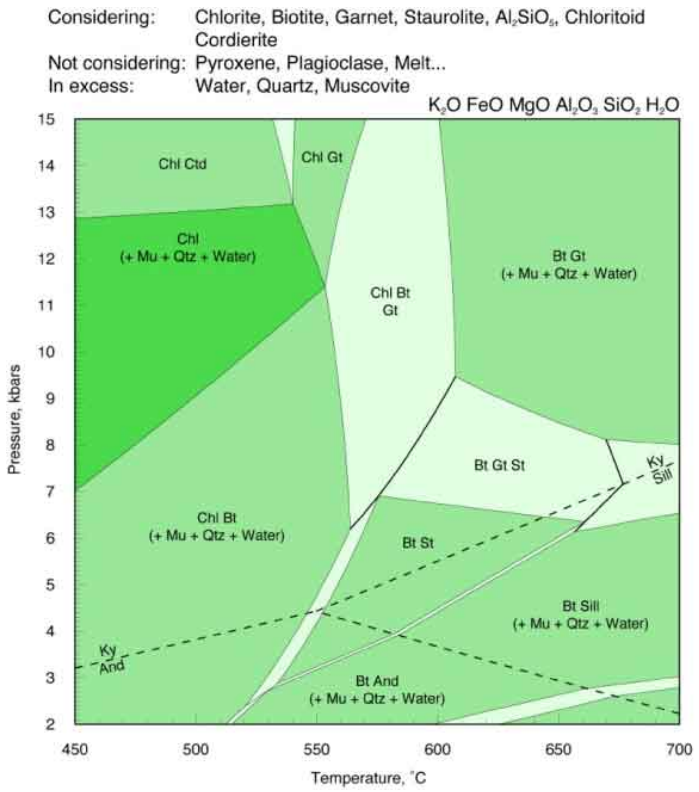
For the Case of Phase Assemblage Diagram Calculations

	THERMOCALC	Perple_X	Theriak-Domino
I want to build this line-by-line, so I really understand the outcome	✔	✘	✘
I don't have the patience for that! I want automation	✘	✔	✔
How long will I be interacting with the program before I get my diagram?	Hours for each diagram (depends on experience)	A few minutes for each diagram*	Not many minutes for each diagram*
How long will the program be calculating in the background without me having to steer it?	–	• 30 seconds (simple thermo' system) • Many hours (complex system)	• A few minutes (simple thermo' system) • 1-6 hours (complex system) • Days (worst case)
Can this time be reduced	Get more experience!	✔ / ✘ (adaptive refinement, parallelization)	–

* But not really

For the Case of Phase Assemblage Diagram Calculations

	THERMOCALC	Perple_X	Theriak-Domino
Will my diagram be publication-ready without editing in a graphics package?	✔ / ✘	✘	✔ / ✘
How easy and time-consuming is contouring modal proportions and compositions of phases?	Time consuming	Very easy & fast	Easy, but repetitive (pixel maps are easier than contour plots)
What about fractionation of phases out of the system?	Straightforward but time consuming	Very easy to do, but also easy to introduce errors*	Straightforward
Might I unintentionally end up with a metastable phase diagram?	✔	✘ (generally)	✘ (generally)
Can I intentionally explore metastable configurations	✔	-	✔
Can I easily map out *G*, *V*, *S*, μ, etc across my diagram?	✘	✔	✔
Would each code give me the same diagram?	?	?	?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Cordierite
Not considering: Pyroxene, Plagioclase, Melt...
In excess: Water, Quartz, Muscovite
K_2O FeO MgO Al_2O_3 SiO_2 H_2O
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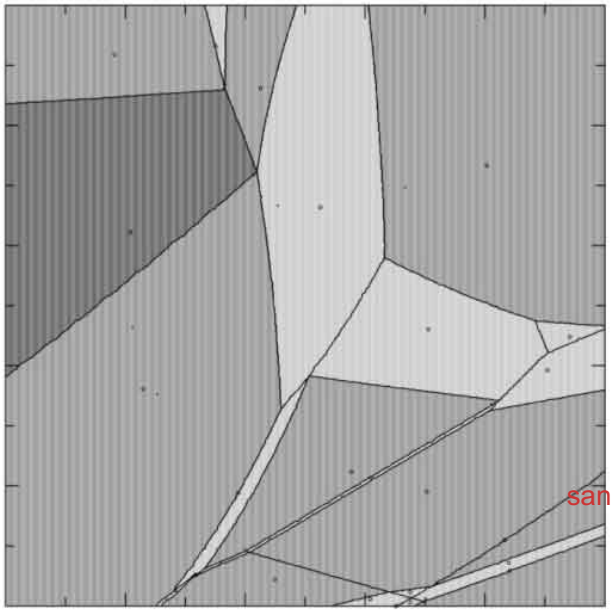
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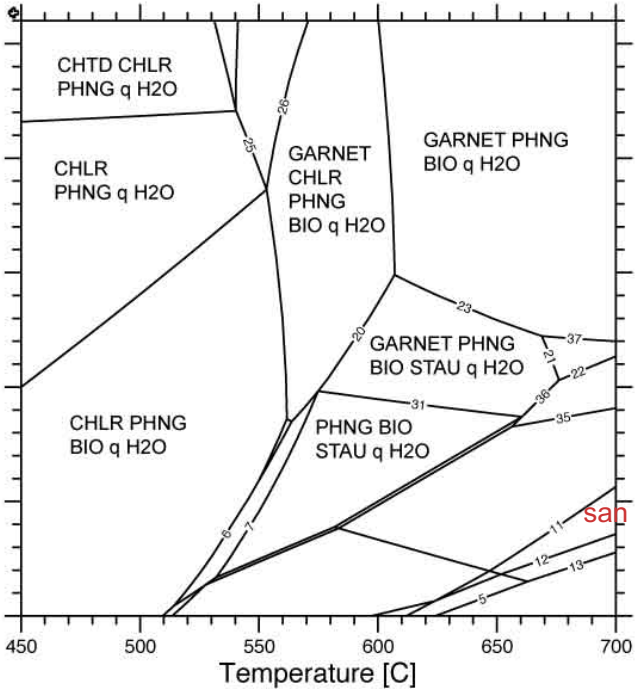
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STAU q H2O
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Temperature [C]

For the Case of Phase Assemblage Diagram Calculations

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Can I easily map out *G*, *V*, *S*, μ, etc across my diagram?	✘	✔	✔
Would each code give me the same diagram?	?	?	?

For the Case of Phase Assemblage Diagram Calculations

	THERMOCALC	Perple_X	Theriak-Domino
• Will my diagram be 'correct'? • Will it be a good description of my rock? • Will I be able to interpret it to solve something important?	?	?	?