title

THERMOCALC Short Course: São Paulo
30 June to 3 July, 2006

taught by *Roger Powell* and *Richard White*,
University of Melbourne

with help from *Dave Kelsey* (University of Adelaide) and
Johann Diener (University of Melbourne)

welcome!

to the 7th THERMOCALC course

- 1. Blacksburg, 2001
- 2. Barcelona, 2002
- 3. Pavia, 2002
- 4. ETH, Zürich, 2003
- 5. Melbourne, 2003
- 6. ETH, Zürich, 2004.

acknowledgements

most obviously:

- my partner in the methodology, Tim Holland (University of Cambridge)
- my main collaborator in applications, Richard White (University of Melbourne)
- and also, currently, Julie Baldwin (University of Montana, Missoula), Pavla Štípská (Université Louis Pasteur, Strasbourg), Gisella Rebay (Universitá di Pavia), Jian-Jun Yang (Chinese Academy of Sciences, Beijing), and Geoff Clarke (University of Sydney), as well as our students.

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- Richard White (co-presenter), and helpers Dave Kelsey and Johann Diener
- previous helpers on the course, particularly Gisella Rebay
- course organisers (Renato Moraes and Mike Brown).

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- the lecture notes (.pdf files like this one) will be part of the material to copy from the course CD. . .

starting point (1)

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- equilibration is strongly promoted by the presence of fluid or melt
- and/or equilibration is promoted by recrystallisation (e.g. as a consequence of deformation)
- preservation of metamorphic mineral assemblages is related primarily to where fluid or melt runs out (in the absence of deformation).

starting point (2)

- *if* this equilibrium model of metamorphism is true, *then* we can identify mineral assemblages/compositions that represent a preserved equilibrium,
- then we can use calculations based on equilibrium thermodynamics to understand metamorphic processes and determine conditions of formation of rocks
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- mineral equilibria modelling only after, and only as good as, field geology/petrography/mineral chemistry (maps)/ geochronology. . .
- this course concerns mineral equilibria modelling using the *thermo*dynamic *calc*ulator, THERMOCALC,
- with a focus on the sort of phase diagrams called pseudosections.

approaches in mineral equilibria modelling

- inverse modelling

- forward modelling

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- inverse modelling
    - make observations on rocks (e.g. identify mineral assemblage; determine mineral compositions, look at composition zoning)
    - thermobarometry, to determine conditions of formation (P, T, fluid composition; $P - T$ paths etc)
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  - thermobarometry, to determine conditions of formation (P, T, fluid composition; $P - T$ paths etc)
- forward modelling
  - of rocks: use rock composition (so overlap with inverse modelling) to draw pseudosections to consider specific processes (and also can be for thermobarometry)
  - of processes: use generalised rock compositions (like average pelite or MORB) to draw pseudosections to consider processes (like preservation of mineral assemblages and dehydration of subducted oceanic crust) .

thermobarometry

to be covered on Day 4, but types of thermobarometry include

- single reaction ("directly-calibrated")
- multiple reaction (based on an internally-consistent dataset)
- calculated pseudosections

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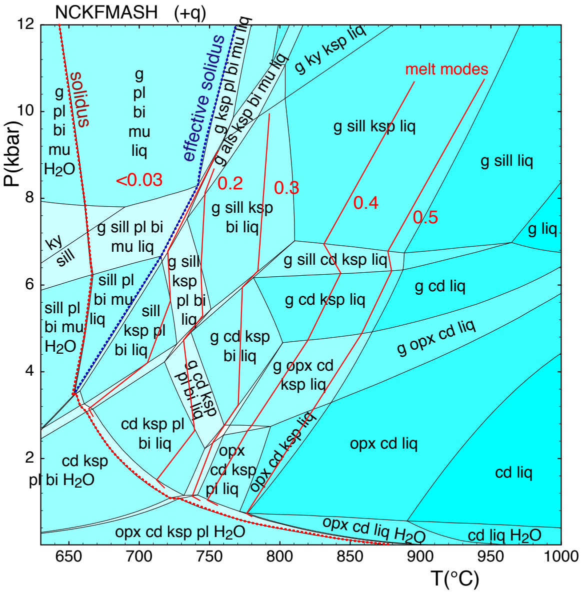
    - mineral stability fields
    - mineral proportion isopleths
    - mineral composition isopleths.

calculating phase diagrams (1)

our main focus, at least on the first 3 days of this Short Course, will be on calculating the sort of phase diagrams called pseudosections

example *PT* pseudosection



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- so you can do the practicals!

- two main aspects to this
    - understanding the geometry of phase diagrams, and
    - understanding how to calculate them with THERMOCALC.

some technical terms (1)

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- phases: minerals, melt, aqueous solutions. . .

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  - composition represented by components, and
  - by end-members that have the same stoichiometry as the phase.

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- the word, system, is also used in the sense of the physicochemical setup being modelled.

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  - reactions that relate *phases*, as might be seen in a texture and on some phase diagrams. These include so-called univariant reactions.
  - reactions that relate *end-members* of phases. These are effectively a thermodynamic construct—we use independent sets of such reactions in various ways—but they do not normally correspond to reactions between actual phases.

some technical terms (4)

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  - ...although there is some argument about whether this is good usage.

what do we need for mineral equilibria modelling?

- thermodynamic descriptions of the phases

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- software that implements the calculation methods.

thermodynamic descriptions of the phases (1)

- *essential* idea:
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- *essential* idea:
  - the extrapolation of experimental data on mineral properties and mineral equilibria in P, T and composition
- how to do this:
  - use equilibrium thermodynamics, as well as statistics. And common sense!

thermodynamic descriptions of the phases (2)

- in the THERMOCALC context, the thermodynamic descriptions are provided
    - the end-member properties in the dataset file
    - the *a*-*x* relationships in each datafile (for a rock, system. . .)

thermodynamic descriptions of the phases (2)

- in the THERMOCALC context, the thermodynamic descriptions are provided
  - the end-member properties in the dataset file
  - the *a*-*x* relationships in each datafile (for a rock, system. . .)
- development is a technical subject, particularly of *a*-*x* relationships
- if you want to find out more about this, the best plan is to read the relevant literature (not all of which is very approachable!)

references for end-member properties

- Powell, R, & Holland, TJB, 1985 An internally consistent thermodynamic dataset with uncertainties and correlations : 1. Methods and a worked example. *Journal of Metamorphic Geology* **3**, 327–342.
- Holland, TJB, & Powell, R, 1985 An internally consistent thermodynamic dataset with uncertainties and correlations : 2. Data and results. *Journal of Metamorphic Geology* **3**, 343–370.
- Holland, TJB, & Powell, R, 1990 An enlarged and updated internally consistent thermodynamic dataset with uncertainties and correlations: the system K_2O-Na_2O-CaO-MgO-MnO-FeO-Fe_2O_3-Al_2O_3-TiO_2-SiO_2-C-H_2-O_2. *Journal of Metamorphic Geology* **8**, 89–124.
- Powell, R, & Holland, TJB, 1993. Is Least Squares an appropriate methodology to be used in the extraction of thermodynamic data from experimentally-bracketed mineral equilibria? *American Mineralogist*, **78**, 107–112.
- Holland, TJB, & Powell, R, 1998. An internally-consistent thermodynamic dataset for phases of petrological interest. *Journal of Metamorphic Geology* **16**, 309–344.

references for *a-x* relationships

- Powell, R, & Holland, TJB, 1993. On the formulation of simple mixing models for complex phases *American Mineralogist* **78**, 1174–1180.
- Holland, TJB, & Powell, R, 1996. Thermodynamics of order–disorder in minerals. 1: symmetric formalism applied to minerals of fixed composition. *American Mineralogist* **81**, 1413–1424.
- Holland, TJB, & Powell, R, 1996. Thermodynamics of order–disorder in minerals. 2: symmetric formalism applied to solid solutions.. *American Mineralogist* **81**, 1425–1437
- Powell, R, & Holland, TJB, 1999. Relating formulations of the thermodynamics of mineral solid solutions: activity modelling of pyroxenes, amphiboles and micas. *American Mineralogist* **84**, 1–14
- Holland, TJB, & Powell, R, 2003. Activity–composition relations for phases in petrological calculations: an asymmetric multicomponent formulation. *Contributions to Mineralogy and Petrology* **145**, 492–501.

what do we need for mineral equilibria modelling? (1)

repeating this

- thermodynamic descriptions of the phases
- for pseudosections, the “bulk” composition of the rock being considered (or, strictly, the composition of an equilibrium volume)

“bulk” composition for pseudosections

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- difficulty/impossibility of scaling down from the chemical analysis of the “real” system to the model system
- . . .
- but progress can be made—with care—and with an eye to the sensitivity of the results to assumptions made.

what do we need for mineral equilibria modelling? (2)

repeating again

- thermodynamic descriptions of the phases
- for pseudosections, the “bulk” composition of the rock being considered (or, strictly, the composition of an equilibrium volume)
- calculation methods for the different sorts of phase diagrams
- software that implements the calculation methods.

methods and software

two competing approaches (methods → software)

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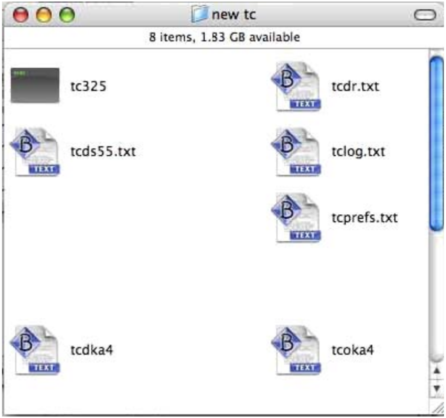
    - e.g. Jamie Connolly's Perplex
- non-linear equation solver
    - locates field boundaries
    - (currently) manual assembly of diagrams, having gained the information line-by-line
    - THERMOCALC.

THERMOCALC

so let's meet THERMOCALC (the Mac and PC versions have the same setup and filenames)



new tc

8 items, 1.83 GB available

tc325

tcdr.txt

tcds55.txt

tclog.txt

tcprefs.txt

tcdka4

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input

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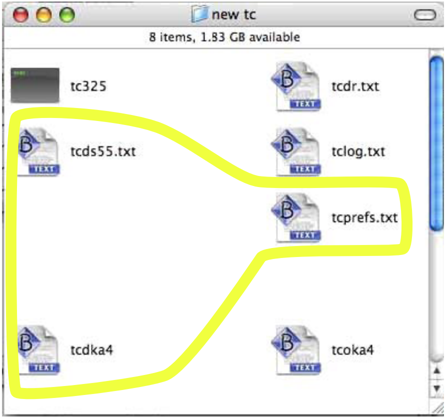
- *tcds55.txt*, the file of the thermodynamic properties of the end-members of phases
- *tcdblah.txt*, where *blah* is your chosen filename, that contains the *a*-*x* relationships of the phases, scripts (that allow you to control how THERMOCALC runs with this file), including things like the bulk composition for a pseudosection.

THERMOCALC

input files



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- *tcdr.txt*, containing, after a THERMOCALC run, the results that can be assembled for drawpd to plot the phase diagram.

THERMOCALC

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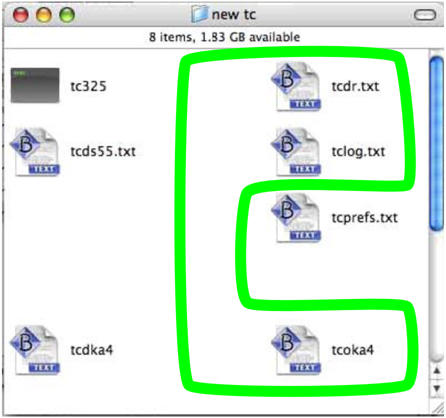

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telling THERMOCALC what to calculate is controlled by

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telling THERMOCALC what to calculate is controlled by

- prompts on screen (i.e. question and answer), but also
- scripts (controlling behaviour, controlling access to facilities, providing short-cuts—simplifying/by-passing prompts—etc)
  - global scripts (in "tcprefs.txt")
  - local scripts (in "tcdblah.txt").

THERMOCALC calculation modes

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- mode 3: for calculations not involving solid solutions (for grids, but also for forms of thermobarometry involving looking at individual reactions between end-members)
- mode 4: for getting the formulae of end-members in the dataset.

good practice in running THERMOCALC?

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- THERMOCALC is set to overwrite the output files each time you fire up the app (although this can be overridden in *tcprefs.txt*)
- a good way to proceed is to have a file called, say, *oblah.txt* into which you copy key results (annotating them if need be) from *tcoblah.txt* or *tclog.txt* after each THERMOCALC run. (The latter is good if you want to record what you did).

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- it is often better to rerun equilibria to collect this drawing information *after* you know what the phase diagram looks like

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- it is often better to rerun equilibria to collect this drawing information *after* you know what the phase diagram looks like
- it is usually more efficient to build up (parts of) the phase diagram on paper—just qualitatively (you don't need graph paper)— before using drawpd.