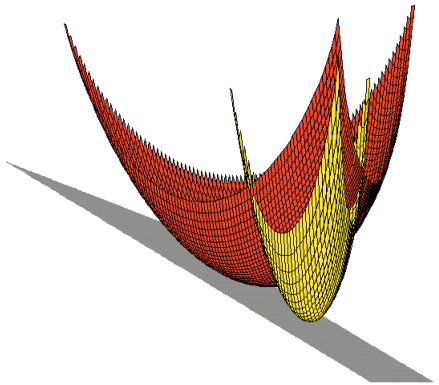

Teaching Petrology and Geochemistry with MELTS software

Current Applications and Future Possibilities

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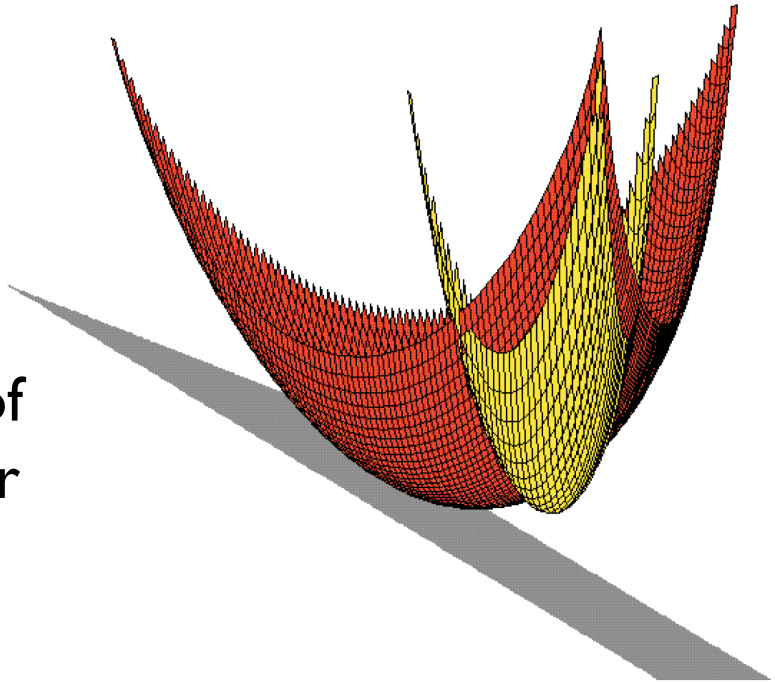
What is MELTS (*sensu lato*)?

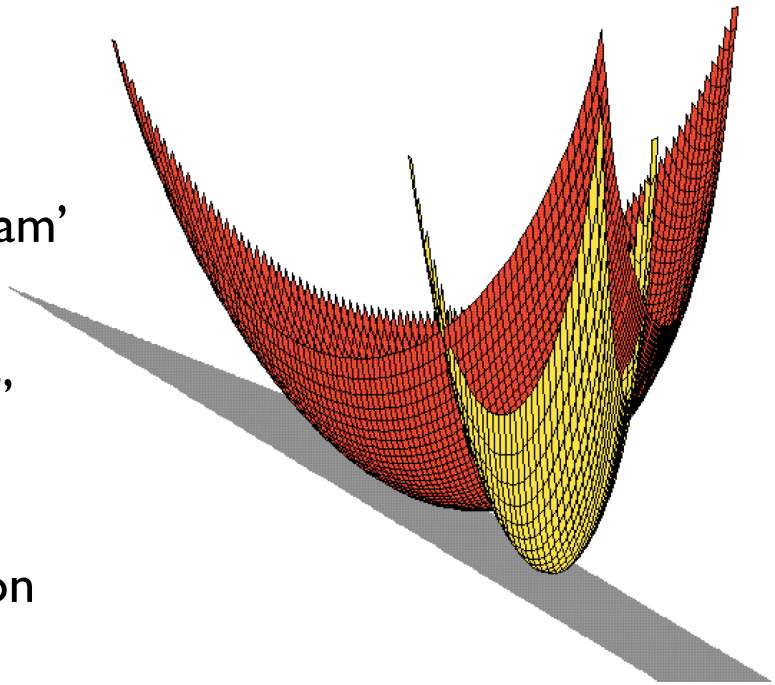
- A family of software packages for modeling phase equilibria in magmatic systems
  - Berman 1988 based database
  - Published solution models for solid phases (& water)
  - Various liquid calibrations (MELTS, pMELTS, …)
- MELTS uses minimization of total free energy (for *PT*) or rather than solving for coincident tangent planes
- GUI and text-based versions
  - http://melts.ofm-research.org/
  - http://magmasource.caltech.edu/



From Ghiorso 1994, GCA 58, 5489-5501

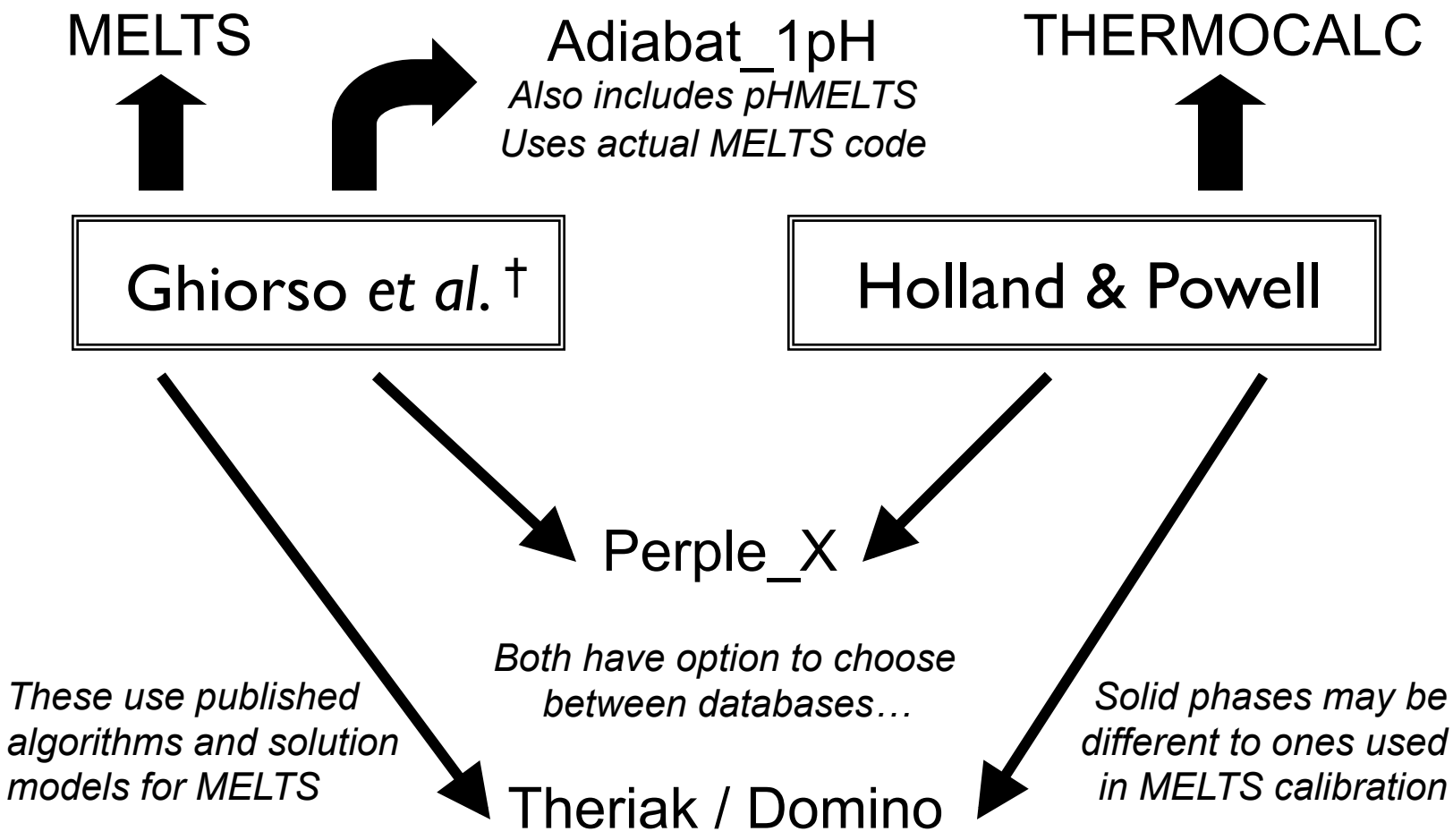
The MELTS family continued

- All MELTS software has capability to do
  - Prescribed *P-T* paths
  - Adiabatic (isentropic)
  - Heat-balanced (isenthalpic)
  - Constant volume (isochoric)
  - 'Find Liquidus' or 'Phase diagram'
  - fO_2 constraints
  - Output includes compositions, thermodynamic data…
- Suitable for e.g.
  - Fractional / batch crystallization and AFC
  - Mantle melting, melt extraction…
- Known issues and limitations
  - See e.g. Hirschmann et al. (1988)



From Ghiorso 1994, GCA 58, 5489-5501

Available thermodynamic software*



* List is not exhaustive e.g. Pele is a Windows clone of MELTS

† Also TWEEQ software (Berman) but no liquid end-members

What is MELTS (liquid model)?

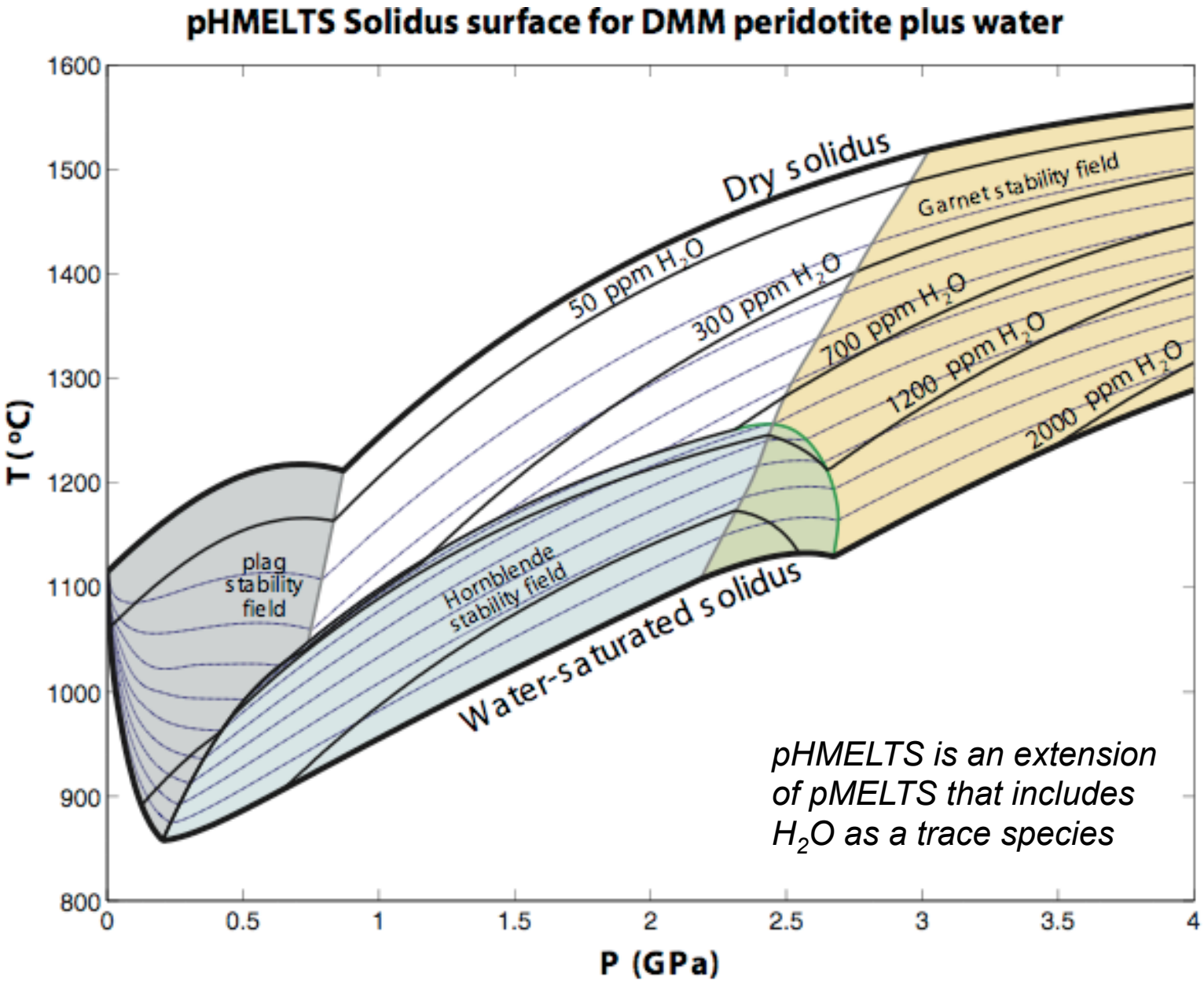
- Ghiorso & Sack (1995) liquid calibration
  - SiO_2-TiO_2-Al_2O_3-Fe_2O_3-Cr_2O_3-FeO-MnO-MgO-NiO-CoO-CaO-Na_2O-K_2O-P_2O_5-H_2O
  - 1 bar – 3 GPa
  - Wide range of bulk compositions but best suited to crystallisation of MORB and alkali basalts
    - H_2O included but relatively few hydrous phases
  - Hornblende and biotite not well modelled
    - Avoid silica-rich calc-alkaline systems
  - Solid end-members and solutions at:

What is pMELTS (liquid model)?

- Ghiorso *et al.* (2002)
  - SiO_2-TiO_2-Al_2O_3-Fe_2O_3-Cr_2O_3-FeO-MgO-CaO-Na_2O-K_2O-P_2O_5-H_2O
  - 1 GPa – 4 GPa
  - Best suited to melting of peridotite bulk compositions
    - H_2O included but few phases to partition into so no solidus at most conditions
    - Pressure limit imposes limits on the mantle potential temperature that can be modeled (e.g. MOR is fine, a mantle plume like Hawaii is not)

What is pHMELTS?

- Asimow *et al.* (2004)
  - Partitioning of H_2O into nominally anhydrous minerals
  - Based on MELTS or pMELTS so same composition and pressure range
  - Best suited for modelling melting of hydrous and water-undersaturated peridotites using pMELTS + H model
  - Can model fractional crystallisation using MELTS + H but rarely required
  - Extra iteration (may be slower on old machines) and not available in GUI



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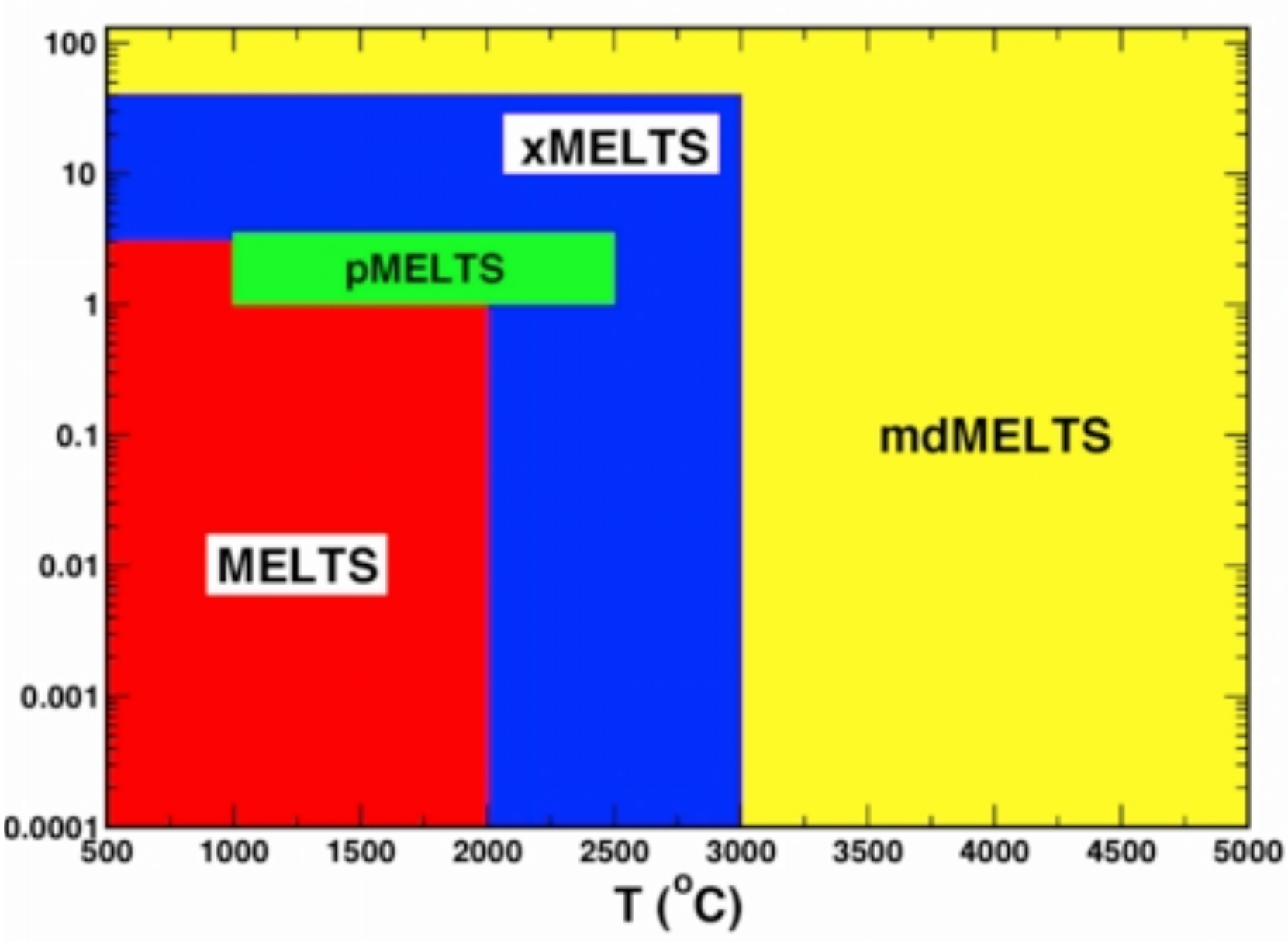
What is Rhyolite-MELTS?

- Gualda *et al.* (submitted 2011)
  - Based on MELTS with adjustments to quartz and kspar (separate download)
  - Best suited for hydrous silicic systems at moderately high melt fractions
    - Not suitable for intermediate compositions with hornblende or biotite
  - Various improvement to underlying algorithms that may eventually transfer
    - e.g. detection of phase saturation routines modified
  - Available for Mac and Linux, GUI only
    - http://melts.ofm-research.org/macosx-rhyolite.html

What is xMELTS?



What is xMELTS?

- xMELTS will eventually be a replacement for MELTS and pMELTS software
  - Will extend modeling capabilities to the top of the Earth's lower mantle (to 40 GPa)
    - Incorporates a new liquid equation of state (EOS)
    - New liquid solution model will extend range of liquid compositions that can be modeled
    - Current work to improve *solid* solution models before finalization of liquid model
  - Associated 'Library of Experimental Phase Relations' is available at:
    - http://lepr.ofm-research.org/

Links to references

- Ghiorso & Sack (1995)
  - CMP, v119, p197-212, DOI: 10.1007/BF00307281
- Ghiorso *et al.* (2002)
  - G-cubed, v3, 1030, DOI:10.1029/2001GC000217
- Asimow *et al.* (2004)
  - G-cubed, v5, Q01E16, DOI:10.1029/2003GC000568
- Gualda, Ghiorso, Lemons, & Carley (2011)
  - Rhyolite-MELTS: A modified calibration of MELTS optimized for silica-rich, fluid-bearing magmatic systems. Submitted to J. Pet., April 14, 2011.
- Ghiorso, and Ghiorso & Kress (2004)
  - Am. J. Sci. v304, nos 8-9 (4 papers on xMELTS EOS)

What is MELTS (front-end)?

- A standalone graphical user interface is available for Mac and Linux
  - MELTS and pMELTS liquid models available
  - Up to date versions only for Leopard onwards on Mac, plus Linux
  - Not available for Windows
  - Double-click (or open terminal to start)
  - *The graphics buttons do not work anymore!*
- http://melts.ofm-research.org/index.html
  - http://melts.ofm-research.org/macosx.html
  - http://melts.ofm-research.org/unix.html

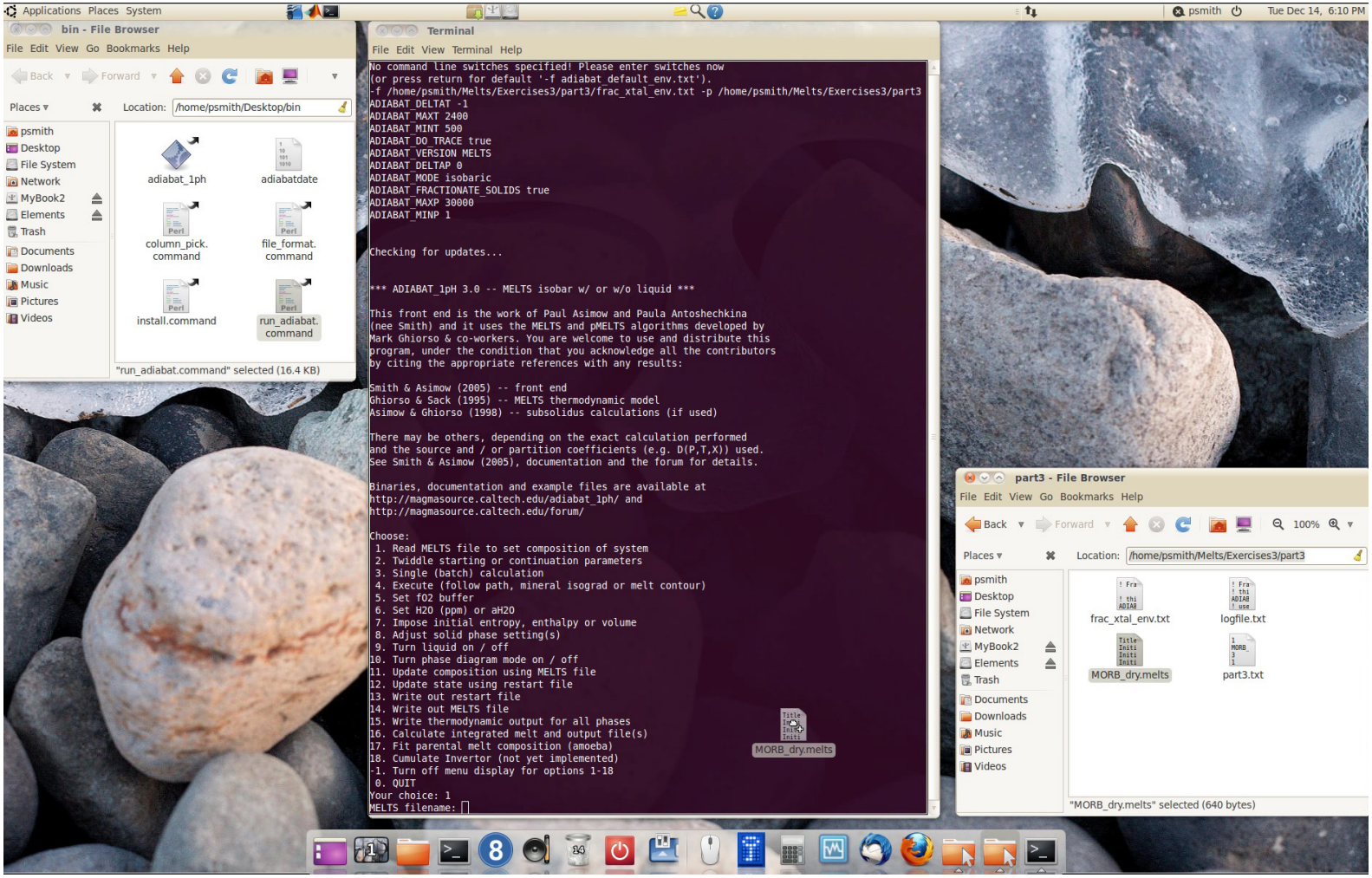
Standalone MELTS GUI

What is Java / Corba MELTS?

- Java MELTS web based applet
  - MELTS and pMELTS models are available
  - Limited functionality / problems with firewalls
  - Now depreciated
- Corba MELTS
  - Mimics standalone GUI more closely
  - MELTS liquid model only
  - Can be slow if server load is heavy
  - http://ctserver.ofm-research.org/MELTS.html
- Can be used on Mac, Linux, Windows
  - Also supplemental calculators

What is Adiabat_1ph?

- A text-based front-end to MELTS
  - MELTS, pMELTS and pHMELTS liquid models
  - Perl scripts included in package for
    - Processing files, settings and running adiabat_1ph
    - Also installation and extracting text output
  - Available for Mac, Linux and Windows
    - On all platforms, suitable input files can be used to automate as much or little of process as desired
  - See Smith & Asimow (2005) software brief:
    - G-cubed, v6, Q02004, DOI:10.1029/2004GC000816
    - Supplemented by AGU Fall meeting presentations:
      - Antoshechkina & Asimow (2010)
      - Antoshechkina et al. (2010)



- Adiabat_1ph 3 was released August, 2011
  - Much more user-friendly than previous (research tool) versions
  - Can double-click all scripts and drag-and-drop files
  - Menus reorganized and less 'kitchen-sink' settings

Adiabat_1ph 3

- Additional features (not in GUI)
  - pHMELTS model or buffer aH_2O
  - More extensive 'phase diagram' mode
  - Trace elements, including D(*P*, *T*, *X*)
  - Radiogenic and stable isotopes
  - Aggregate fractional melts and bulk crust
  - Some 'supplemental calculator' like output
  - 'Reverse' fractionation and 'amoeba routines'
  - Lots of documentation (also useful for GUI)
  - Forum and tutorials (work in progress) for Adiabat_1ph and MELTS GUI on same site

MELTS and Adiabat_1ph Users

USER INFO

Welcome, **Guest**. Please login or register.
Did you miss your activation email?
Registering will give you access to more of the forum's features as well as (optional) e-mail notification of future Adiabat_1ph releases. Please enter the e-mail address at which you would like to be contacted.
December 14, 2010, 06:02:02 pm

Search: Search Advanced search

HOME | DOWNLOAD | HELP | SEARCH | LOGIN | REGISTER

NEWS BOX

Welcome to the users' forum for MELTS and Adiabat_1ph! The current Adiabat_1ph software, version **2.0.1**, is available at the download and information site.

KEY STATS

144 Posts in **50** Topics by **92** Members
Latest Member: **waza**

MELTS and Adiabat_1ph Users

General Forum

News and updates Latest software releases, updates and changes to this or other Caltech **MAGMA** sites. If you are new to this forum then *please read this first!*	10 Posts in 10 Topics	Last post on September 14, 2009, 03:06:41 am in The forum has moved! by Paula
Website issues Comments or queries about using this forum or other Caltech **MAGMA** sites. Also please report any download problems here.	9 Posts in 3 Topics	Last post on March 24, 2010, 02:40:07 am in Re: downloading version ... by Daniel Fröhlich
Community Announcements Whether you are convening a meeting session or looking to hire a postdoc, if you have a posting that might be of interest to other forum users then you may share it here.	0 Posts in 0 Topics	
Miscellaneous Feel free to talk about anything and everything that doesn't fit elsewhere. Also post here if you're not sure which board your message should be on.	0 Posts in 0 Topics	

MELTS and Adiabat_1ph

Scientific discussion Comments or queries about results of MELTS or Adiabat_1ph calculations. Want to draw attention to a recent study that used MELTS? Post an abstract or link here.	0 Posts in 0 Topics	
MELTS, pMELTS and pHMELTS algorithms Anything to do with the underlying algorithms, including the thermodynamic calibrations and experimental database. Also the next generation MELTS model: xMELTS.	4 Posts in 3 Topics	Last post on September 18, 2009, 01:52:19 pm in Mineral phases available... by Paula
Interactive operation Using MELTS or Adiabat_1ph to model specific geological settings. *Child Boards: General usage, Melting processes, Magma chamber processes*	52 Posts in 14 Topics	Last post on July 07, 2010, 11:01:06 am in Re: Assimilation followe... by Paula
Technical details Front-end issues for GUI or Adiabat_1ph versions of MELTS, including input and output file formats, specifying options etc.. *Child Boards: MELTS GUI, Adiabat_1ph & run_adiabat.pl*	45 Posts in 14 Topics	Last post on July 21, 2009, 03:52:25 pm in Re: Continuous fractiona... by Paula
Operating system specific Issues that affect users of a particular operating system. *Child Boards: Windows, Linux, MacOS X*	18 Posts in 4 Topics	Last post on November 22, 2010, 10:22:39 am in Re: Melts Graphics Outpu... by Paula
Software tools, support and development A place to share tips and add-ons, such as scripts for plotting results. We welcome any comments or feedback about the software too and will try to accommodate suggestions. *Child Boards: Tips, tools & add-ons, Bug reports, Feature requests*	6 Posts in 2 Topics	Last post on September 17, 2009, 04:54:49 pm in Reading Excel data into ... by Paula

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The **MAGMA** website (http://magmasource.caltech.edu/) at **Caltech** is an online resource for the study of mantle melting and magma evolution, which includes:

- **MELTS and Adiabat_1ph Users forum**
- **Adiabat_1ph software download and information site**
- **Geodynamics: integration of melt formation and migration into mantle flow models**
- **Movies of phase diagrams for adiabatic decompression melting of peridotite and pyroxenite sources**
- **Applet for visualization of binary phase diagrams, tutorial and downloadable software for ternary version**

- **Source** code, scripts and examples
- ... plus **links** to other useful sites.

The MAGMA website includes links to the Adiabat_1ph download site and forum:

- http://magmasource.caltech.edu/adiabat_1ph/
- http://magmasource.caltech.edu/forum/

Available MELTS software

	GUI	JavaMELTS	CorbaMELTS	Adiabat_Iph
MELTS	Yes	Yes	Yes	Yes
pMELTS	Yes	Yes	No	Yes
pHMELTS	No	No	No	Yes
rhyMELTS	Yes	No	No	No

	GUI	JavaMELTS	CorbaMELTS	Adiabat_Iph
Mac PPC	Somewhat	Somewhat *	Yes	Yes
Mac Intel	Yes	Somewhat	Yes	Yes
Linux	Yes	Somewhat	Yes	Yes
Windows	No	Somewhat	Yes	Yes

* 'Somewhat' is used to indicate that software is available but not actively maintained

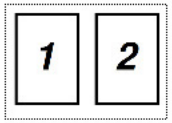
The good, the bad and the ugly

- Opportunity to hypothesis test
- Limitations of model
  - Effect of minor components
  - Uncertainties in calibrated experiments
- Complex modelling software can become something of a black box. Possibilities:
  - Relate to phase diagrams (e.g. *T-X* or *S-X*)?
  - Relate to real datasets (as extended project)?
  - Synthetic data with noise and other strategies
- Data manipulation and operating system
  - MELTS / Adiabat_1ph program failures

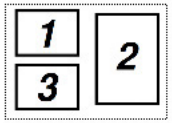
Relate MELTS to phase diagrams

Please go to the Movie Home Page for information about the available options:

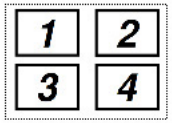
Layout:



2 movies



3 movies



4 movies

1/2 page layout

Movie 1:

Plot axes: P-T

System: Fo-En

Source type: Heterogeneous (perid + pyrox)

Mixing ratio: Normal

Melt regime: Fractional

Copy options

Movie 2:

Plot axes: S-X

System: Fo-En

Source type: Heterogeneous (perid + pyrox)

Mixing ratio: Normal

Melt regime: Fractional

Copy options

Movie 3:

Plot axes: Melt fraction

System: Fo-En

Source type: Heterogeneous (perid + pyrox)

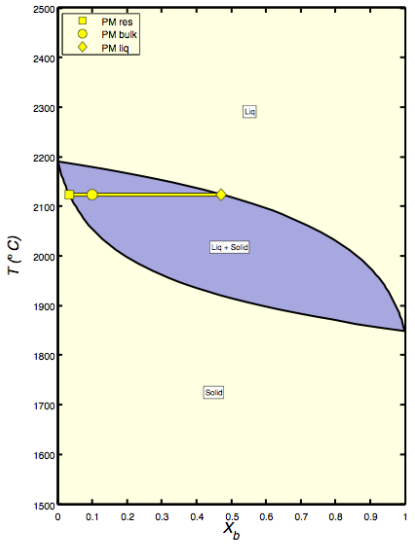
Mixing ratio: Normal

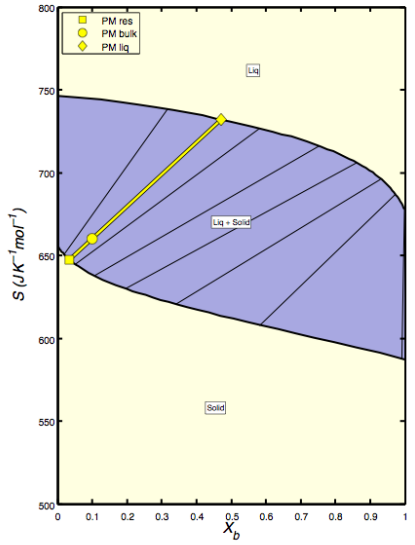
Melt regime: Fractional

Copy options

Output will be in this window by default. Ctrl-click or Shift-click will open a new window or tab:

Submit and play | Submit and download | Submit and print | Save query | Reset | No frames





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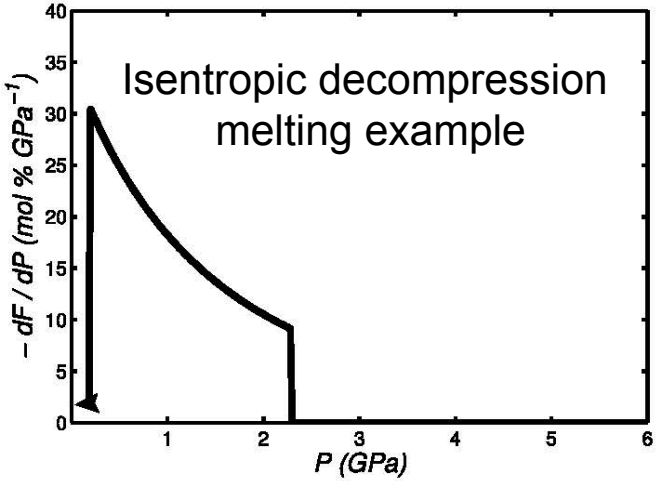
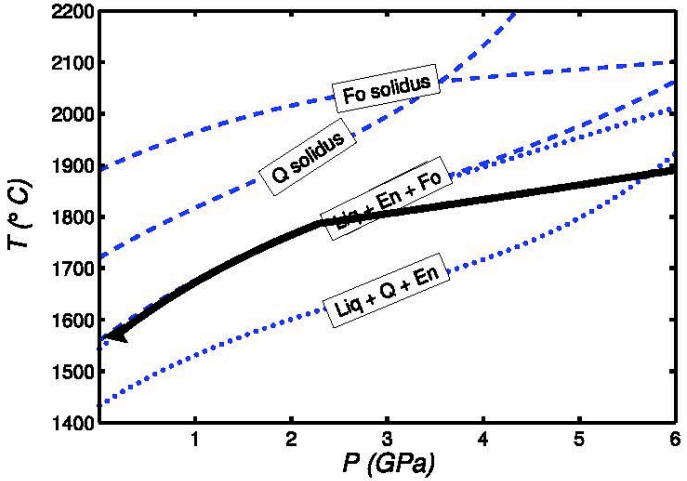
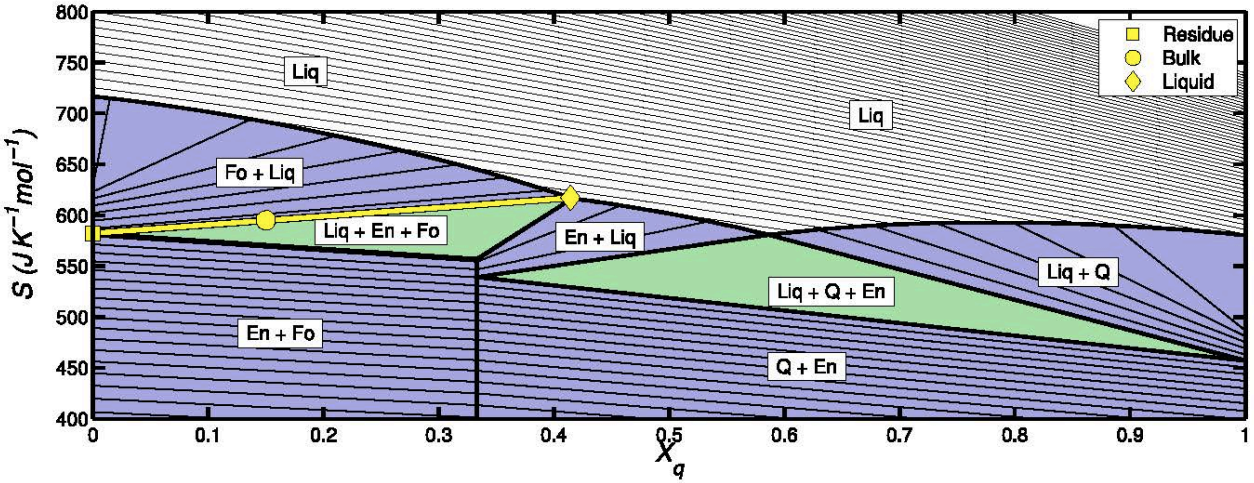
Relate MELTS to phase diagrams







http://magmasource.caltech.edu/movies/

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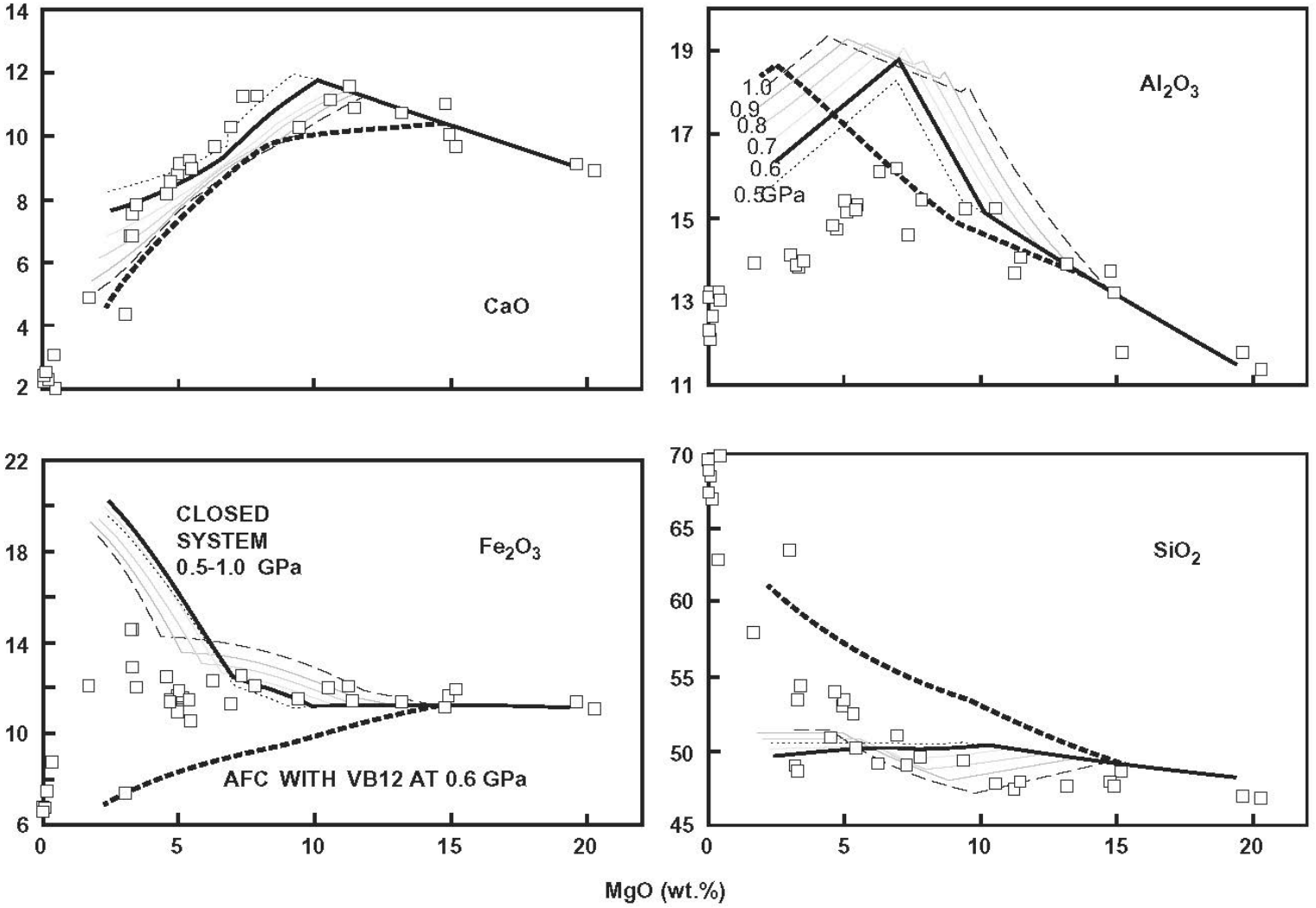
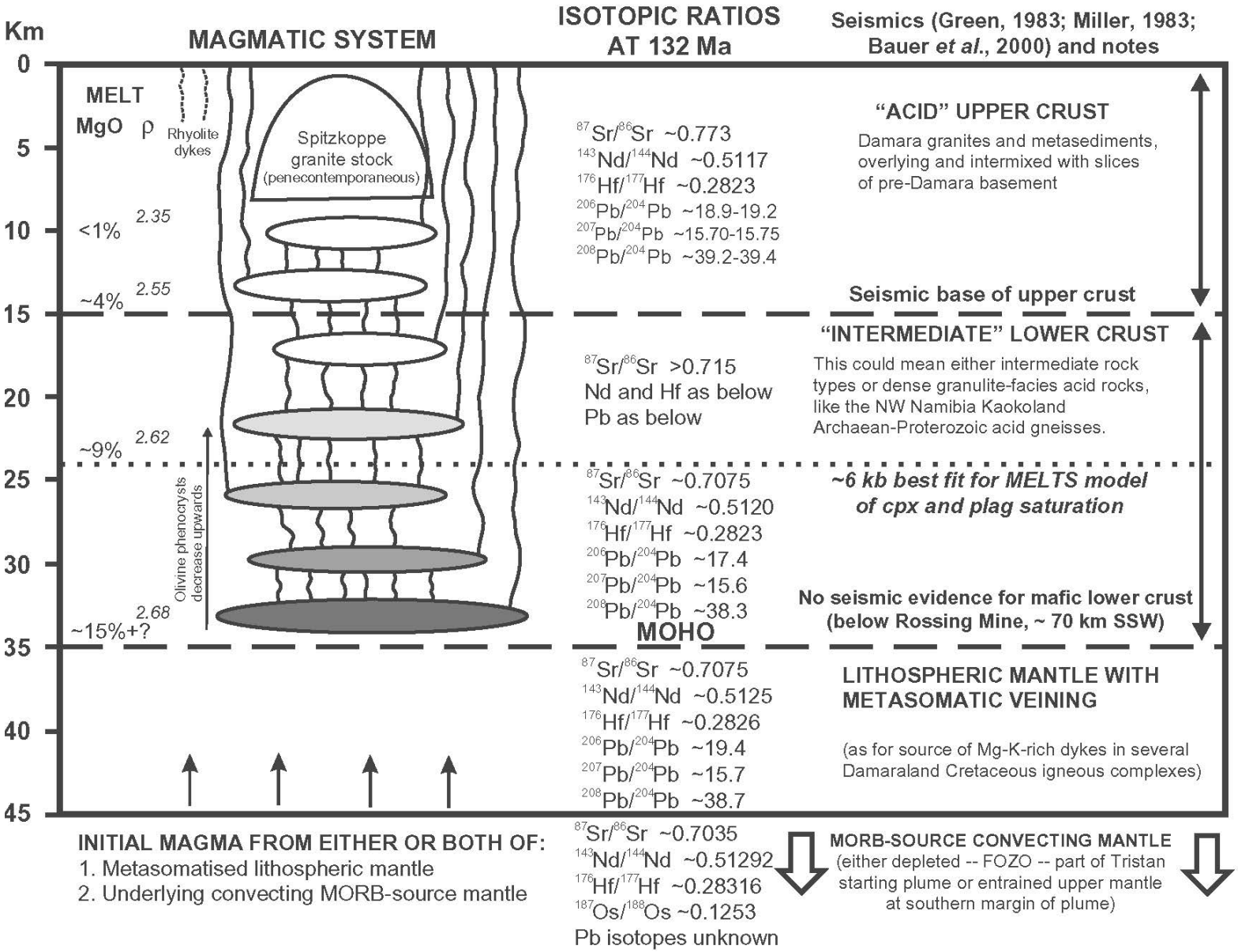
Real world examples



Testing fractional crystallization at various P versus AFC, using local rocks for assimilant

From Thompson et al. (2007)

Real world examples



- ‘Life before MELTS was completely different from life after MELTS.’
- ‘I fully understand the limitations of MELTS but… it lets me test petrogenetic hypotheses… in an incredible variety of igneous environments.’
- ‘… porting it to Windows so I don't any longer need to buy and maintain a special Linux computer solely for running MELTS, … I can (and do) use it as a teaching tool and encourage my graduate students to use it to test their ideas.’ (*Referring to Adiabat_1ph 2 which is less user-friendly*)
- ‘I think one of the things that has not been well appreciated by the geochemical community is the degree to which we can now model trace elements and isotopes together with thermodynamically consistent phase equilibria.’

Future work

- More tutorials and teaching activities
  - E.g. for pMELTS, pHMELTS, Rhyolite-MELTS
- xMELTS development
  - Improve solid solutions (e.g. spinel volume model, and add more components to garnet and pyroxene)
  - Finalize liquid calibration and release software
- Hydrous phases
  - Finish chlorite and add biotite in similar way
  - Hornblende is more complicated (needs more experiments?)
- MatlabMELTS (intended mainly as research tool)
  - Will be able to query activity models directly
  - More flexibility with partition coefficients etc.

Your questions and suggestions

- How to extract data easily?
  - column_pick.command, part of the Adiabat_1ph package, can be used to select, align and pad data from multiple files to make a single text file
  - Could be used to collect results from a class if, say, each student is given different *P-T* conditions to use
- Older versions of MELTS plotted AFM diagrams?
  - Current MELTS software does not plot any graphs
  - IgPet is available for a fee and is easy to use
  - We need a free alternative for Excel users
  - Ternary Plots is available from the Matlab File Exchange
- Can MELTS be used as a 'virtual laboratory'?
  - Yes, and compared with http://lepr.ofm-research.org/