

PERPLE_X TUTORIALS

This set of 13 tutorials has been prepared to teach students how to use Perple_X to make different types of phase diagrams. This is the practical part of a 30 hours advanced course on “Petrologic phase diagrams: principles and computations” periodically offered to PhD students by Daniele Castelli and Chiara Groppo (Dept. of Earth Sciences, University of Torino, Italy).

All the calculations have been performed with **Perple_X version 6.9.1** (released on January 14, 2022). Each tutorial consists of a pdf file with the commented dialogs and a folder containing all the files produced during calculation. The perplex_option.dat file used for each calculation is provided in the corresponding folders.

The exercises should be done **sequentially**, following the order indicated by the numbers. Most of the prompts are, in fact, explained only the first time they appear and comments are not repeated later.

Topics addressed in the 13 exercises are as follows:

Understanding the differences between projections, chemographies and pseudosections

Ex 1: P-T projection for the Al_2SiO_5 system

Pag. 4

This exercise explains how to calculate a P-T projection for the very simple, two-components system $SiO_2-Al_2O_3$ (quartz in excess), showing phase relations among the three alumino-silicate polymorphs. The influence of different thermodynamic databases on the position of the And-Ky-Sil triple point is also explored.

Ex 2: P-T projection for the CMSH system (no solid solutions)

Pag. 16

This exercise explains how to calculate a P-T projection for the very simple CMSH system; the grid shows all the possible equilibria for this system in the P-T range 200-1000°C, 0.5-20 kbar.

Ex 3: Composition diagrams (chemographies) for the CMSH system

Pag. 30

This exercise explains how to calculate composition diagrams (i.e. chemographies) for the P-T projection of Ex. 2, at specified P-T conditions.

Ex 4: P-T pseudosection for the CMSH system (no solid solutions)

Pag. 41

This exercise explains how to calculate a very simple pseudosection, not involving solid solutions. Combined with Ex. 2 and Ex. 3, this exercise is useful to understand the difference between P-T projections and P-T pseudosections.

Ex 5: T-X(CO_2) projections and pseudosections for the CMS- H_2O-CO_2 system (no solid solutions)

Pag. 54

This exercise investigates prograde metamorphism of impure dolomites and limestones characterized by different amounts of Cal, Dol and Qtz. A constant pressure of 1 kbar, typical of shallow level contact aureoles, is considered. This exercise is useful to understand the difference between T-X(CO_2) projections and T-X(CO_2) pseudosections and allows you to become familiar with the use of H_2O-CO_2 fluids.

Working with solid solutions

Ex 6: T-XMg section for the CaCO₃-MgCO₃ system (solvus relations)

Pag. 87

This exercise explains how to calculate **solvus relations** in the system CaCO₃-MgCO₃. In this system two miscibility gaps exist, and the phases on either side of the gaps are calcite/dolomite, and dolomite/magnesite, respectively. The amounts of MgCO₃ in calcite in equilibrium with dolomite, and that of CaCO₃ in magnesite in equilibrium with dolomite, change as a function of temperature, and can be used as geothermometers. The effect of pressure on the Cal-Dol and Dol-Mag *solvi* is investigated by calculating the same phase diagram at different pressures.

Ex 7: P-T projection for the CaCO₃-MgCO₃ system using solid solutions

Pag. 101

This exercise explains how to calculate a P-T projection for the CaCO₃-MgCO₃ system, using solid solutions (rather than end members only). Combined with Ex. 6, this exercise provides the opportunity for understanding the relationships between isobaric T-X sections and P-T projections.

Working with solid solutions in a more complex system

Ex 8: AFM chemographies in the KFMASH system

Pag. 117

This exercise explains how to calculate the “classical” Thompson AFM diagrams for metapelites in the KFMASH system. Opposite to Ex. 3, solid solutions are here considered. The concept of **COMPONENT TRANSFORMATION** is introduced in order to create the three new components: MU = 0.5 K₂O + 1.5 Al₂O₃, PHL = 1.5 MgO – 0.5Al₂O₃ and ANN = 1.5 FeO – 0.5Al₂O₃.

Ex 9: P-T pseudosection for a METAPELITE in the KFMASH system

Pag. 130

This exercise explains how to calculate a P-T pseudosection for a metapelite sample in the simplified KFMASH system, using solid solutions. The influence of other components (Na₂O, CaO and MnO) will be considered in the next exercise (Ex. 10). At the end, some **PRACTICAL TIPS FOR REDRAWING** the PerpleX outputs are given, and the comparison with the AFM chemographies calculated in Ex. 8 will be done. The second part of this exercise explains **how to calculate ISOMODES and compositional ISOPLETHS**.

Ex 10: P-T pseudosection for a METAPELITE in the MnNKCFMASH system

Pag. 161

This exercise is intended to explore the influence of some minor components (Na₂O, CaO and MnO) on the topology of the pseudosection calculated for the metapelite sample investigated in Ex. 9. The exercise also explains **how to calculate CUMULATIVE MODES ALONG A GEOTHERMAL GRADIENT**.

Ex 11: T-XMg pseudosection for a METAPELITE in the MnNKCFMASH system

Pag. 171

This exercise is intended to explore the influence of bulk XMg [MgO/(MgO+FeO)] on the stability fields of the main mineral assemblages, for the same metapelite sample investigated in Ex. 9 and 10. The exercise provides the opportunity to calculate an isobaric T-X pseudosection (i.e. a phase diagram section with a compositional parameter on the horizontal axis).

Modelling a melt-bearing system

Ex 12: DIRECT modelling of an anatectic METAPELITE (NKCFMASH system)

Pag. 180

This exercise deals with the “DIRECT” modelling of a metapelite sample at supra-*solidus* conditions (i.e. melt-bearing). “Direct modelling” means that you know which is the protolith composition, including its initial H₂O amount (which is generally not the case).

Ex 13: INDIRECT modelling of an anatectic METAPELITE (NKCFMASH system)

Pag. 196

This exercise explains the strategy for modelling a REAL SAMPLE OF ANATECTIC METAPELITE, i.e. a metapelite whose protolith is unknown, and that has lost some melt during prograde metamorphism.

Ex 1

Ex. 1 – P-T projection for the Al₂SiO₅ system

This exercise explains how to calculate a P-T diagram for the very simple, two-components system SiO₂-Al₂O₃ (quartz in excess), showing phase relations among the three aluminosilicate polymorphs.

The influence of different thermodynamic databases on the position of the And-Ky-Sil triple point is also explored.

(1) Definition of the problem (BUILD)

```
C:\PERPLEX\Perplex691>build
```

Perple_X version 6.9.1, source updated January 3, 2022.

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NO is the default (blank) answer to all Y/N prompts

Enter a name for this project (the name will be used as the root for all output file names) [default = my_project]:

Here you specify the name of your project.

Project names should not include blanks or "." characters, but they may include directory information. The project name can be up to 100 characters long, but because output files are named using project name plus various suffixes (e.g., .dat, .plt, .prt, .arf, .tof, .tab) it is unwise to specify names that are longer than 93 characters.

ex1

The problem definition file will be named: ex1.dat

Enter thermodynamic data file name [default = hp02ver.dat]:

The HP (Holland & Powell) databases are the most used in metamorphic petrology. In this exercise we will use the hp02 (Holland & Powell, 1998, revised 2002). We will then compare the results with that obtained using the more recent hp62 database (from the THERMOCALC version TC-DS62; Holland & Powell, 2011).

More information about the HP databases are given at <https://hpxeosandthermocalc.org/the-hpx-eos/hp02ver.dat>

Enter the computational option file name [default = perplex_option.dat]:

See: www.perplex.ethz.ch/perplex_options.html

Here you can press ENTER. The perplex_option.dat file specifies some computational parameters that Perple_X uses to make the calculations: **it is better NOT to modify these parameters, at least at the beginning.**

Explanations for each of these parameters are at: http://www.perplex.ethz.ch/perplex_options.html

Reading Perple_X options from: perplex_option.dat

The current data base components are:

NA2O MGO AL2O3 SIO2 K2O CAO TIO2 MNO FEO NIO ZRO2 CL2 O2 H2O CO2

Transform them (Y/N)?

n

This is the lists of the **CHEMICAL COMPONENTS** considered in the chosen database.

This option would permit the user to redefine the database components, e.g., to create Fe₂O₃ from the components FeO and O₂ (i.e. Fe₂O₃ = 2FeO + 0.5 O₂).

Component transformations in BUILD are tedious, so if you are going to do many calculations with transformed components, the program CTRANSF can be used to create a thermodynamic data file with transformed components.

Specify computational mode:

- 1 - Convex-Hull minimization
- 2 - Constrained minimization on a 2d grid [default]
- 3 - Constrained minimization on a 1d grid
- 4 - Output pseudocompound data
- 5 - 1-d Phase fractionation
- 6 - 0-d Infiltration-reaction-fractionation
- 7 - 2-d Phase fractionation (FRAC2D and TITRATE reactive transport models)

Use Convex-Hull minimization for Schreinemakers projections or phase diagrams with > 2 independent variables. Use constrained minimization for phase diagrams or phase diagram sections with < 3 independent variables.

1

Use option 1 (Convex-Hull minimization) for PROJECTIONS (Schreinemakers-type diagrams) or CHEMOGRAPHIES (composition diagrams; phase diagrams with > 2 independent variables). Use options 2 or 3 (Constrained minimization on a 2d grid/1d grid) for PSEUDOSECTIONS (phase diagrams or phase diagram sections with < 3 independent variables).

Calculations with a saturated fluid (Y/N)?

n

Fluid is not considered in this specific calculation, because reactions among alumino-silicates are solid-solid reactions.

Calculations with saturated components (Y/N)?

SATURATED COMPONENTS are components whose chemical potentials are determined by the assumed stability of a pure phase consisting entirely of a saturated component, e.g., a system that contains so much silica that a silica polymorph (e.g., quartz or coesite) is stable at all conditions of interest can be specified here by selecting SiO₂ as a saturated component.

NB. If more than one saturated component is specified, Perple_X applies the constraints sequentially, e.g., if Al₂O₃ and SiO₂ are specified as the first and second components, then the excess phases might be corundum + andalusite, if the order is reversed then, at the same conditions, the stable phases would be quartz + andalusite. This sequence is referred to as the **saturation hierarchy**.

y

****warning ver015**** if you select > 1 saturated component, then the order you enter the components determines the saturation heirarchy and may effect your results (see Connolly 1990).

Select < 6 saturated components from the set:

NA₂O MGO AL₂O₃ SiO₂ K₂O CAO TIO₂ MNO FEO NIO ZRO₂ CL₂ O₂ H₂O CO₂

Enter names, 1 per line, press <enter> to finish:

SiO₂

(NB. It is CASE-SENSITIVE!).

Use chemical potentials, activities or fugacities as independent variables (Y/N)?

N

The answer would be Y if you want to calculate a phase diagram with chemical potentials (μ), activities or fugacities on one (or on both) axes (e.g. T-log f_{O_2} phase diagrams).

Select thermodynamic components from the set:

NA2O MGO AL2O3 K2O CAO TIO2 MNO FEO NIO ZRO2 CL2 O2 H2O CO2

Enter names, 1 per line, press <enter> to finish:

AL2O3

Here is where you specify the components for your system.

THERMODYNAMIC COMPONENTS are components whose chemical potentials are the dependent (implicit) variables of a phase diagram calculation. **Phase diagram calculations require the specification of at least one thermodynamic component.**

The data base has P(bar) and T(K) as default independent potentials.

Make one dependent on the other, e.g., as along a geothermal gradient (y/n)?

N

The answer would be Y if you want to consider a geothermal gradient along an axes, rather than P or T.

Specify number of independent potential variables:

0 - Composition diagram [default]

1 - Mixed-variable diagram

2 - Sections and Schreinemakers-type diagrams

2

0 = chemografies (*see Ex3*);

1 = T-X or P-X diagrams (e.g. T-XMgO)

2= classical phase diagram projections and sections.

Select x-axis variable:

1 - P(bar)

2 - T(K)

2

Enter minimum and maximum values, respectively, for: T(K)

473

1073

T is expressed in Kelvin

Enter minimum and maximum values, respectively, for: P(bar)

1000

12000

P is expressed in bar

Output a print file (Y/N)?

Y

Exclude pure and/or endmember phases (Y/N)?

N

Here you can specify if you want to exclude some phases from the calculation.

Include solution models (Y/N)?

N

Solid solutions are not considered, because we are modelling reactions between end-member phases.

Enter calculation title:

ex1

This name appears at the top of the diagram.

After finishing with BUILD, a .dat file is generated within the Perple_X folder. This new file (named ex1.dat) is the input file for the following calculation steps.

(2) Doing the calculation (CONVEX)

Run CONVEX to make the calculation:

```
C:\PERPLEX\Perplex691>convex
```

Perple_X version 6.9.1, source updated January 3, 2022.

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Enter the project name (the name assigned in BUILD) [default = my_project]:

ex1

This section summarizes where CONVEX reads the input data (thermodynamic database, input file generated with build etc.), and where CONVEX writes the results (print output, plot output).

Reading problem definition from file: ex1.dat

Reading thermodynamic data from file: hp02ver.dat

Writing print output to file: ex1.plt

Writing plot output to file: ex1.plt

Reading solution models from file: not requested

Reading Perple_X options from: perplex_option.dat

Writing complete reaction list to: not requested

Writing Perple_X option summary to: not requested

This section summarizes all the parameters (“computational option settings”) used in the calculation and specified in the perplex_option.dat file.

Perple_X computational option settings for CONVEX:

Keyword: Value: Permitted values [default]:

Auto-refine options:

auto_refine aut [auto] manual off

replicate_threshold 0.1E-1 [1e-2]; static opt; <0 => no replica test

rep_dynamic_threshold 0.1E-2 [1d-3]; dynamic opt; <0 => no replica test

re-refine F [F] T

intermediate_savrpc F [F] T

intermediate_savdyn F [F] T

keep_all_rpcs T [T] F

Schreinemakers and Mixed-variable diagram options:

variance 1/99 [1/99], >0; maximum true variance
increment 0.100/0.025 [0.1/0.025], default search/trace variable increment
efficiency 3 [3] >0, <6
reaction_format min [min] full stoichiometry S+V everything
reaction_list off [off] on
console_messages on [on] off
short_print_file on [on] off

Solution subdivision options:

initial_resolution:
exploratory stage 0.0625 0->1 [1/16], 0 => off
auto-refine stage 0.0208 0->1 [], 0 => off
stretch_factor 0.0020 >0 [2d-3]
non_linear_switch F [F] T
subdivision_override off [off] lin str
hard_limits off [off] on
refine_endmembers F [F] T
pc_perturbation 0.0050 [5d-3]

Thermodynamic options:

solvus_tolerance aut [aut] or 0->1; aut = automatic, 0 => p=c pseudocompounds, 1 => homogenize
T_stop (K) 0.0 [0]
T_melt (K) 873.0 [873]
approx_alpha T [T] F
Anderson-Gruneisen F [F] T
speciation_precision 0.1E-4 [1d-5] <1; absolute
speciation_max_it 100 [100]
GFSM F [F] T GFSM/special_component toggle
hybrid_EoS_H2O 4 [4] 0-2, 4-7
hybrid_EoS_CO2 4 [4] 0-4, 7
hybrid_EoS_CH4 0 [0] 0-1, 7
aq_bad_results err [err] 101 102 103 ignore
aq_lagged_speciation F [F] T
aq_ion_H+ T [T] F => use OH-
aq_oxide_components F [F] T
aq_solvent_solvus T [T] F
aq_vapor_epsilon 1.0 [1.]

Input/Output options:

pause_on_error T [T] F
timing T [T] F
auto_exclude T [T] F

To change these options see: www.perplex.ethz.ch/perplex_options.html

The calculation starts here:

Summary of make-definition entities:

sil8L q8L

Summary of saturated-component entities:

```
for: SIO2
q   trd   crst   coe   stv   qL   qGL   q8L
```

```
-----
** Starting auto_refine computational stage **
Initial number of divariant assemblages to be tested is:  1
Testing divariant assemblage  1,  0 assemblages remaining to be tested.
finished with equilibrium (  1) ky = and
finished with equilibrium (  2) ky = sill
finished with equilibrium (  3) and = sill
Testing divariant assemblage  2,  0 assemblages remaining to be tested.
Testing divariant assemblage  3,  0 assemblages remaining to be tested.
Testing divariant assemblage  4,  0 assemblages remaining to be tested.
```

At the end, you have two new files in the Perple_X folder. An ex1.prn file, which is the text file with all the information about the calculation, and an ex1.plt file, that is the plot file.

(3a) Plotting the calculated phase diagram (PSVDRAW)

Run PSVDRAW to plot the calculated phase diagram:

```
C:\PERPLEX\Perplex691>psvdraw
```

Perple_X version 6.9.1, source updated January 3, 2022.

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Enter the project or plot file name [i.e., without the .plt suffix]:

ex1

Perple_X plot options are currently set as:

Keyword:	Value:	Permitted values [default]:
axis_label_scale	1.20	[1.2] (rel)
bounding_box :		
	0	[0] x-min (pts)
	0	[0] y-min (pts)
	800	[800] x-length (pts)
	800	[800] y-length (pts)
field_fill	T	[T] F
field_label	T	[T] F
numeric_field_label	F	[F] T, if T PSSECT writes list to *_assemblages.txt
replicate_label	0.250	0->1 [0.025]
field_label_scale	0.75	[0.72] (rel)
font	Helvetica	
grid	F	[F] T
half_ticks	T	[T] F
line_width	1.00	0-99 [1.] (pts)
picture_transformation :		
	0.180	[0.18] x-scale (rel)
	0.180	[0.18] y-scale (rel)
	130.	[0.18] x-translation (pts)
	220.	[0.18] y-translation (pts)

```

0.00 [0.0] rotation (deg)
plot_aspect_ratio 1.000 [1.0] x_axis_length/y_axis_length
splines          T      [T] F
tenth_ticks      F      [F] T
text_scale       1.000 [1.] (rel)
plot_extra_data

```

To change these options edit or create the plot option file

See: www.perplex.ethz.ch/perplex_plot_options.html

PostScript will be written to file: ex1.ps

Modify the default plot (y/n)?

N

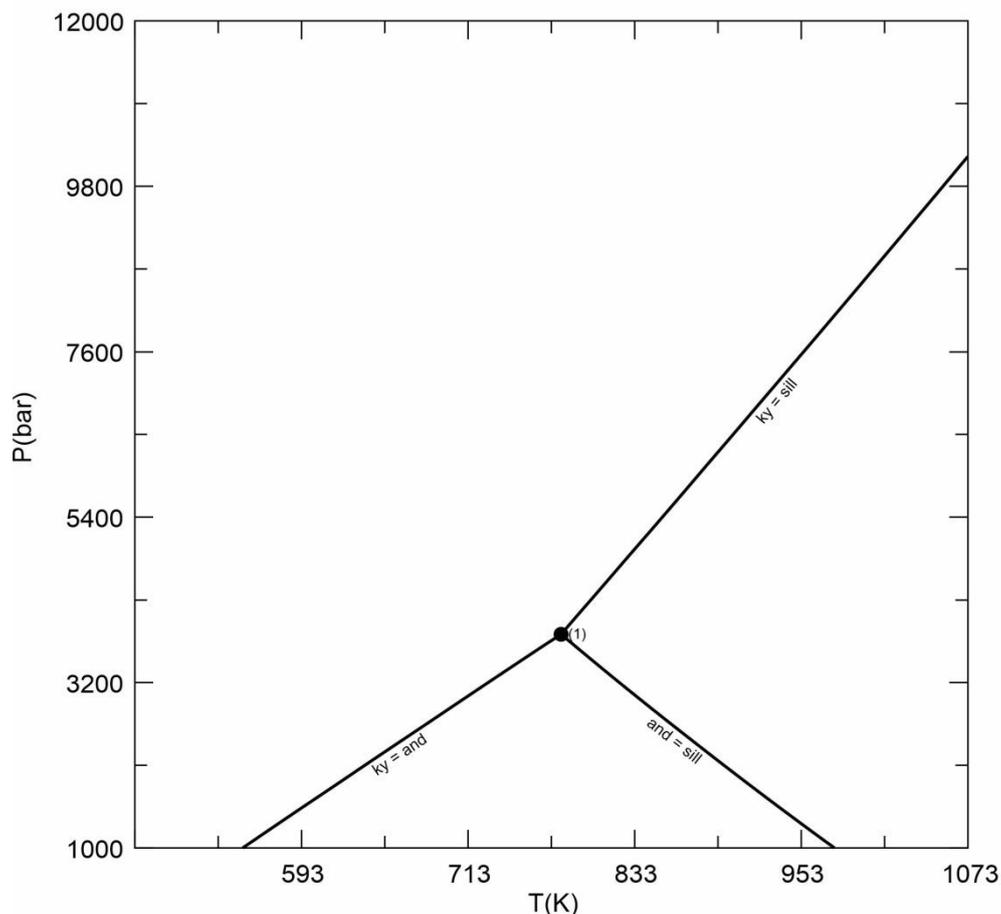
If you replay Y to this prompt, you can change the output, for example you can modify the minimum and maximum T or P along the axes etc. (see below).

At the end, you have a new file ex1.ps in the Perple_X folder. You can open this file with any graphical software (e.g. CorelDraw, Adobe Illustrator etc.) and also convert it in a pdf file.

```

ex1
Component saturation hierarchy: SIO2
Reaction equations are written with the high T(K) assemblage to the right of the = sign

```



The alumino-silicate triple point is modelled at 507°C, 3.8 kbar.

(3b) Modifying the default plotting of the calculated phase diagram (PSVDRAW)

E.g. we want to modify the axes numbering (intervals on x axis = 100°C; intervals on y axis = 2 kbar) and we want to assign a numeric label (rather than a text label) to the reaction curves.

Run again PSVDRAW:

```
C:\PERPLEX\Perplex691>psvdraw
```

Perple_X version 6.9.1, source updated January 3, 2022.

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Enter the project or plot file name [i.e., without the .plt suffix]:

ex1

Perple_X plot options are currently set as:

Keyword:	Value:	Permitted values [default]:
axis_label_scale	1.20	[1.2] (rel)
bounding_box :		
	0	[0] x-min (pts)
	0	[0] y-min (pts)
	800	[800] x-length (pts)
	800	[800] y-length (pts)
field_fill	T	[T] F
field_label	T	[T] F
numeric_field_label	F	[F] T, if T PSSECT writes list to *_assemblages.txt
replicate_label	0.250	0->1 [0.025]
field_label_scale	0.75	[0.72] (rel)
font	Helvetica	
grid	F	[F] T
half_ticks	T	[T] F
line_width	1.00	0-99 [1.] (pts)
picture_transformation :		
	0.180	[0.18] x-scale (rel)
	0.180	[0.18] y-scale (rel)
	130.	[0.18] x-translation (pts)
	220.	[0.18] y-translation (pts)
	0.00	[0.0] rotation (deg)
plot_aspect_ratio	1.000	[1.0] x_axis_length/y_axis_length
splines	T	[T] F
tenth_ticks	F	[F] T
text_scale	1.000	[1.] (rel)
plot_extra_data		

To change these options edit or create the plot option file

See: www.perplex.ethz.ch/perplex_plot_options.html

PostScript will be written to file: ex1.ps

Modify the default plot (y/n)?

y

Modify drafting options (y/n)?

answer yes to modify:

- field labeling
- x-y plotting limits
- axes numbering

y

Modify x-y limits (y/n)?

Answer Y if you want to modify the T and/or P range of the diagram.

n

Restrict phase fields by variance (y/n)?

answer yes to:

- suppress pseudounivariant curves and/or pseudoinvariant points of a specified true variance.

This question is only relevant for more complex calculations, involving solution models and therefore considering also pseudo-univariant curves (i.e. di-variant equilibria involving two pseudocompounds of the same phase as reactant and product). *See Ex. 7.*

n

Restrict phase fields by phase identities (y/n)?

answer yes to:

- show fields that contain a specific assemblage
- show fields that do not contain specified phases
- show fields that contain any of a set of specified phases

n

Modify default equilibrium labeling (y/n)?

answer yes to:

- modify/suppress [pseudo-] univariant curve labels
- suppress [pseudo-] invariant point labels

y

Suppress curve labels (y/n)?

n

Change default labeling of curve segments (y/n)?

y

Suppress labels of pseudounivariant curves (y/n)?

y

Enter minimum fraction of the axes length that a curve must be to receive a text label (0-1):

1 means that a text label will be assigned to those curves that are longer than the axes length.

1

Enter minimum fraction of the axes length that a curve must be to receive a numeric label (0-1.000):

0 means that a numeric label will be assigned to all those curves that are shorter than the axes length.

0

Suppress point labels (y/n)?

n

Modify default axes numbering (y/n)?

y

Enter the starting value and interval for major tick marks on the X-axis (current values are: 473. 120.)

Enter the new values:

473

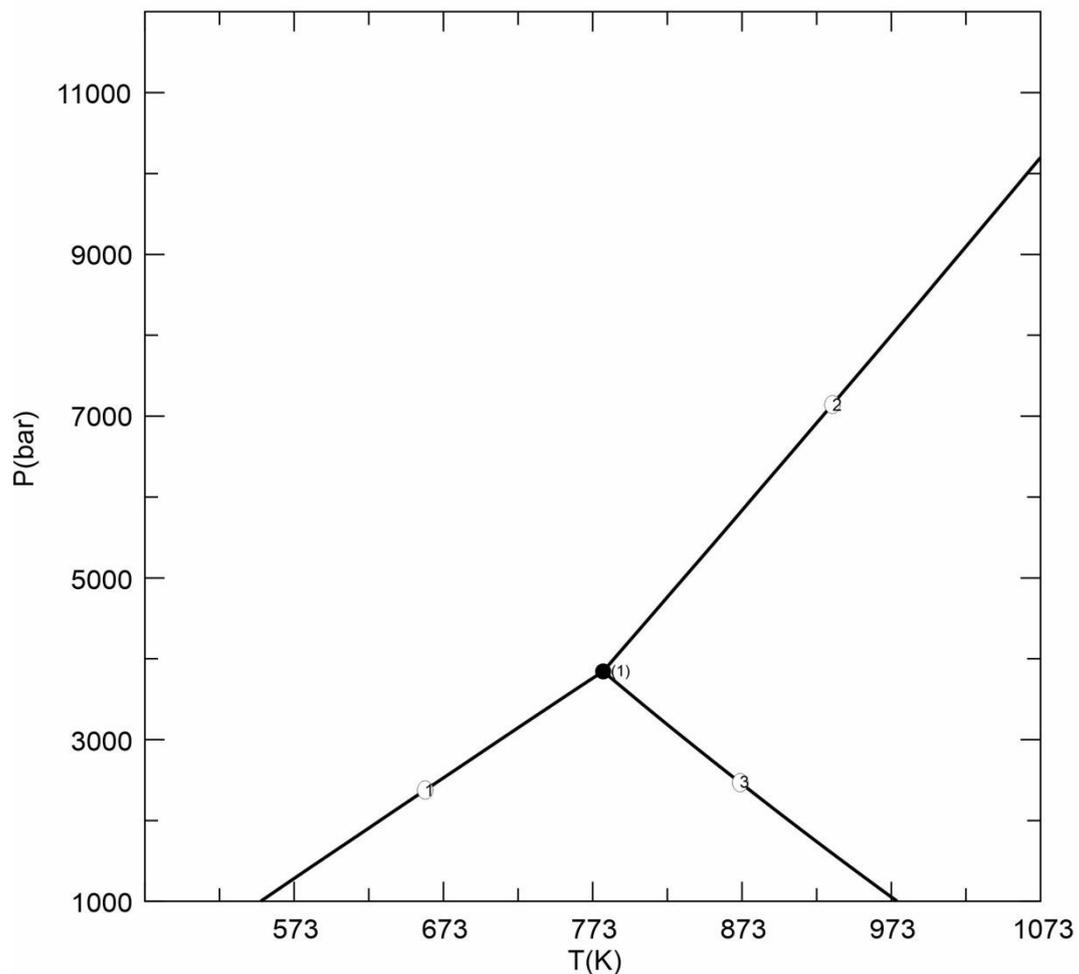
100

Enter the starting value and interval for major tick marks on the Y-axis (current values are: 0.100E+04 0.220E+04)

Enter the new values:

1000

2000



Equilibria corresponding to each reaction number are explained in the ex1.prn file.

(4) Using a different thermodynamic database

In order to test the influence of different thermodynamic databases on the position of the And-Ky-Sil triple point, you can edit the input file previously created using BUILD.

Open the **ex1.dat** input file and change its name in **ex1_hp62.dat**

The thermodynamic database is specified in the first line.

Change **hp02ver.data** to **hp62ver.dat**.

```
hp62ver.dat      thermodynamic data file
```

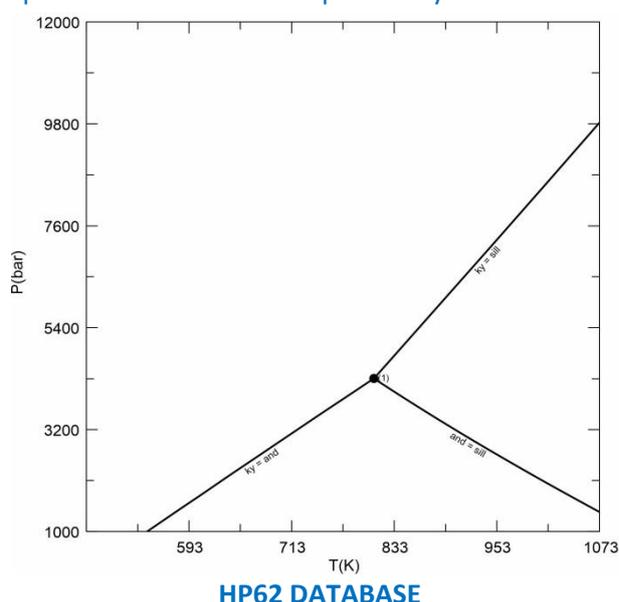
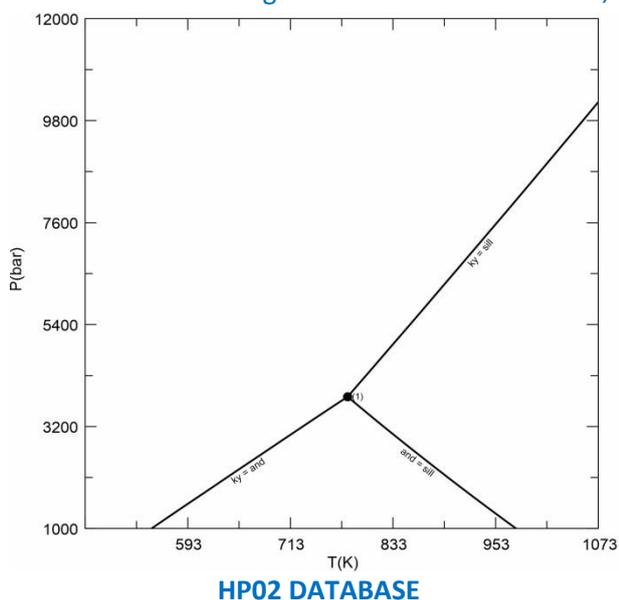
The most recent databases such as hp62ver.dat, define thermodynamic components with both upper and lower case characters (e.g. SiO₂, Al₂O₃ etc.), opposite to the old databases, in which thermodynamic components were defined with upper case characters only (e.g. SIO₂, AL₂O₃ etc.).

In the input file, change the thermodynamic components accordingly.

```
begin thermodynamic component list
Al2O3 0 0.00000      0.00000      0.00000      unconstrained amount
end thermodynamic component list

begin saturated component list
SiO2 0 0.00000      0.00000      0.00000      unconstrained amount
end saturated component list
```

Save the file and run again CONVEX and PSVDRAW; compare the result with that previously obtained.



The alumino-silicate triple point is now modelled at 550°C, 4.4 kbar.

The change in the position of the triple point dates back to the 2004 revision of the HP database. In the 2002 version (hp02ver.dat) the aluminosilicate triple point is at 3.8 kbar and 507 °C, consistent with Holdaway's (1971) estimate; in the 2004 revision (and in the following versions, such as hp62ver.dat) the properties of the aluminosilicates have been adjusted to place the triple point at 4.4 kbar and 550 °C to satisfy a petrological argument of Pattison (1992).

Ex 2

Ex. 2 – P-T projection for the CSMH system (no solid solutions)

This exercise explains how to calculate a P-T projection for the very simple CSMH system; the grid will show all the possible equilibria for this system in the P-T range 200-1000°C, 0.5-20 kbar.

(1) Definition of the problem (BUILD)

```
C:\PERPLEX\Perplex691>build
```

Perple_X version 6.9.1, source updated January 3, 2022.

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NO is the default (blank) answer to all Y/N prompts

Enter a name for this project (the name will be used as the root for all output file names) [default = my_project]:

```
ex2
```

The problem definition file will be named: ex2.dat

Enter thermodynamic data file name [default = hp02ver.dat]:

The HP (Holland & Powell) databases are the most used in metamorphic petrology. One of the most recent HP databases is hp62 from the THERMOCALC version TC-DS62; Holland & Powell, 2011). I suggest using the hp62ver.dat database, which has been tested in the last years and has demonstrated to be reliable for both metapelitic and metabasic systems.

```
hp62ver.dat
```

Enter the computational option file name [default = perplex_option.dat]:

See: www.perplex.ethz.ch/perplex_options.html

```
[ENTER]
```

Reading Perple_X options from: perplex_option.dat

The current data base components are:

Na2O MgO Al2O3 SiO2 K2O CaO TiO2 MnO FeO NiO ZrO2 Cl2 O2 H2O CO2 CuO Cr2O3 S2 F2 N2 ZnO

Transform them (Y/N)?

```
n
```

This is the lists of the **CHEMICAL COMPONENTS** considered in the chosen database.

This option would permit the user to redefine the database components, e.g., to create Fe2O3 from the components FeO and O2 (i.e. $FE2O3 = 2FE0 + 0.5 O2$).

Component transformations in BUILD are tedious, so if you are going to do many calculations with transformed components the program CTRANSF can be used to create a thermodynamic data file with transformed components.

Specify computational mode:

1 - Convex-Hull minimization

2 - Constrained minimization on a 2d grid [default]

- 3 - Constrained minimization on a 1d grid
- 4 - Output pseudocompound data
- 5 - 1-d Phase fractionation
- 6 - 0-d Infiltration-reaction-fractionation
- 7 - 2-d Phase fractionation (FRAC2D and TITRATE reactive transport models)

Use Convex-Hull minimization for Schreinemakers projections or phase diagrams with > 2 independent variables. Use constrained minimization for phase diagrams or phase diagram sections with < 3 independent variables.

1

Use option 1 (Convex-Hull minimization) for PROJECTIONS (Schreinemakers-type diagrams) or CHEMOGRAPHIES (composition diagrams; phase diagrams with > 2 independent variables). Use options 2 or 3 (Constrained minimization on a 2d grid/1d grid) for PSEUDOSECTIONS (phase diagrams or phase diagram sections with < 3 independent variables).

Calculations with a saturated fluid (Y/N)?

Y

There are two important implications to specifying a **SATURATED PHASE**: 1) it implies that the phase components are always present in sufficient quantity to saturate the system in the phase; 2) it implies that the specified phase is always stable. Thus, if you are interested in a system with excess H₂O, but the physical conditions of the system may be those at which ice is stable, you should specify H₂O as a saturated component and not as saturated phase. Similarly, if water may not be always present as a pure phase you should specify H₂O as a thermodynamic component.

In most cases, fluid can be considered as in excess. This means that the user should consider a saturated fluid in the calculation (e.g. H₂O, CO₂ or a mixture of H₂O+CO₂).

NOTE: Because specification of H₂O as a saturated phase component causes Perple_X to exclude any phases with the H₂O composition that are not named "H₂O", H₂O should not be specified as a saturated fluid phase in calculations involving a hydrous silicate melt if, as is commonly the case, the melt model involves a water end-member that is not named "H₂O" (e.g. h₂oL). This means that, for calculations at supra-solidus conditions (e.g. melt-bearing systems), the user must consider H₂O as a normal chemical component, and not as a saturated fluid phase (*see Ex. 12 and Ex. 13*).

Select the independent saturated fluid components:

H₂O CO₂

Enter names, 1 per line, press <enter> to finish:

For C-O-H fluids it is only necessary to select volatile species present in the solids of interest. If the species listed here are H₂O and CO₂, then to constrain O₂ chemical potential to be consistent with C-O-H fluid speciation treat O₂ as a saturated component. Refer to the Perple_X Tutorial for details.

H₂O

Calculations with saturated components (Y/N)?

N

SATURATED COMPONENTS are components whose chemical potentials are determined by the assumed stability of a pure phase consisting entirely of a saturated component, e.g., a system that contains so much silica that a silica polymorph (e.g., quartz or coesite) is stable at all conditions of interest can be specified here by selecting SiO₂ as a saturated component.

If more than one saturated component is specified `Perple_X` applies the constraints sequentially, e.g., if `Al2O3` and `SiO2` are specified as the first and second components, then the excess phases might be corundum + andalusite, if the order is reversed then, at the same conditions, the stable phases would be quartz + andalusite. This sequence is referred to as the **saturation hierarchy**.

Use chemical potentials, activities or fugacities as independent variables (Y/N)?

N

The answer would be Y if you want to calculate a phase diagram with chemical potentials (μ), activities or fugacities on one (or on both) axes (e.g. T- $\log f_{O_2}$ phase diagrams).

Select thermodynamic components from the set:

Na2O MgO Al2O3 SiO2 K2O CaO TiO2 MnO FeO NiO ZrO2 Cl2 O2 CO2 CuO Cr2O3 S2 F2 N2 ZnO

Enter names, 1 per line, press <enter> to finish:

MgO

CaO

SiO2

Because the thermodynamic data file identifies: H2O as special components, you will be prompted next for the EoS to be used for the corresponding components and mixtures thereof. To override this behavior, e.g., to use a generic hybrid fluid EoS, delete the `special_component` section from the thermodynamic data file header.

NOTE: the EoS choice specified here will override the EoS choice specified by the `hybrid_EoS` option, to override this behavior delete the `special_component` section from the the thermodynamic data file header.

Select fluid equation of state:

- 0 - X(CO2) H2O-CO2 Modified Redlich-Kwong (MRK) DeSantis et al 74
- 1 - X(CO2) H2O-CO2 HSMRK Kerrick & Jacobs 81
- 2 - X(CO2) H2O-CO2 MRK hybrid-EoS*
- 5 - X(CO2) H2O-CO2 CORK Holland & Powell 91, 98
- 8 - f(O2/CO2) C-buffered COH MRK hybrid-EoS*
- 10 - X(O) C-buffered COH MRK hybrid-EoS Connolly & Cesare 93*
- 12 - X(O)-f(S2) C-buffered COHS MRK hybrid-EoS Connolly & Cesare 93*
- 13 - X(H2) H2O-H2 MRK hybrid-EoS*
- 14 - X(CO2) H2O-CO2 Pitzer & Sterner 94; Holland & Powell mixing 03
- 15 - X(H2) H2O-H2 low T MRK hybrid-EoS*
- 16 - X(O) H-O MRK hybrid-EoS*
- 17 - X(O)-f(S2) H-O-S MRK hybrid-EoS*
- 19 - X(O)-X(S) C-buffered COHS MRK hybrid-EoS Connolly & Cesare 93*
- 20 - X(O)-X(C) COHS MRK hybrid-EoS Connolly & Cesare 93*
- 24 - f(O2/CO2)-N/C C-buffered COHN MRK hybrid-EoS*
- 25 - X(CO2)-X(NaCl) H2O-CO2-NaCl Aranovich et al 10
- 26 - X(O) O-Si MRK Connolly 16
- 27 - X(O)-X(C) C-O-H MRK hybrid-EoS*

*Hybrid EoS use the following pure species EoS, to change these associations modify the `hybrid_EoS` keywords in the `perplex_option` file:

H2O - PSEoS Pitzer & Sterner 1994

CO2 - PSEoS Pitzer & Sterner 1994

CH4 - MRK DeSantis et al 1974

5

Here you define the **EQUATION OF STATE (EoS) for the fluid phase**.

Most thermodynamic databases are based on equilibria which involve a fluid phase, and are therefore derived with a specific fluid equation of state. When using such databases **it is usually wise to choose (if possible) the fluid EoS used in the data derivation for calculations.** Thus, **the Holland & Powell (1991, 1998) EoS (choice 5) is optimal for the Holland & Powell's databases;** and Kerrick & Jacobs' (1981) equation of state (choice 1) (or the hybrid equations of state, e.g. choices 2, 8 or 10) for Berman's (1988) database. At high pressures above 20 kbar most of the equations of state for water become thermodynamically unrealistic, CORK (choice 5) minimizes this problem.

For rough calculations the differences between the EoS are not important and **in the interest of saving computer time choices 5 and 0 are optimal.** Choices 12-27 are equations of state for multispecies H-O, H-O-S, C-O-H, C-O-H-S and H₂O-CO₂-NaCl fluids.

The data base has P(bar) and T(K) as default independent potentials.

Make one dependent on the other, e.g., as along a geothermal gradient (y/n)?

n

The answer would be Y if you want to consider a geothermal gradient along an axes, rather than P or T.

Specify number of independent potential variables:

- 0 - Composition diagram [default]
- 1 - Mixed-variable diagram
- 2 - Sections and Schreinemakers-type diagrams

2

0 = chemografies;

1 = T-X or P-X diagrams (e.g. T-XMgO)

2= classical phase diagram projections and sections

Select x-axis variable:

- 1 - P(bar)
- 2 - T(K)
- 3 - Y(CO₂)

*Although only one component is specified for the Y(CO₂) phase, its equation of state permits use of its compositional variable:

2

Enter minimum and maximum values, respectively, for: T(K)

473

1273

Select y-axis variable:

- 2 - P(bar)
- 3 - Y(CO₂)

2

Enter minimum and maximum values, respectively, for: P(bar)

500

20000

Specify sectioning value for: Y(CO₂)

0

Having included only H2O as saturated fluid component, XCO2 is 0.

Output a print file (Y/N)?

Y

For unconstrained minimization calculations, particularly mixed-variable diagrams and Schreinemakers projections, **the print file contains a summary of the computed phase equilibria.**

Exclude pure and/or endmember phases (Y/N)?

y

Here you can specify if you want to exclude some phases from the calculation, and if you want to see the list of the mineral phases compatible with your system. The end-member phases are identified by abbreviated names, in general these abbreviations are defined in the header section of the thermodynamic data file. Phases followed by L (e.g. qL) are required for the melt solution and you can therefore exclude them for calculations without melt.

Do you want to be prompted for phases (Y/N)?

n

Enter names, 1 per line, press <enter> to finish:

I suggest excluding the following end-member phases, which are not relevant for this calculation and may result metastable at low-T.

rnk	rankinite Ca3Si2O7
lrn	larnite Ca2SiO4
cstn	"Si-titanite" CaSi2O5 (one Si replaces Ti)
wo	wollastonite CaSiO3
pswo	pseudo-wollastonite CaSiO3
wal	wollastonite CaSiO3
ak	akermanite Ca2MgSi2O7
merw	merwinite Ca3MgSi2O8
mont	monticellite CaMgSiO4
chum	clinohumite Mg9Si4O16(OH)2
cen	clinoenstatite Mg2Si2O6
cumm	cummingtonite Mg7Si8O22(OH)2
cumm_dqf	cummingtonite for Diener et al. (2007) cAmph model
woL	wollastonite LIQUID
limL	lime LIQUID
mcpv	make definitions for Holland et al., 2013 mantle mineralogical model
cmpv	make definitions for Holland et al., 2013 mantle mineralogical model
cpv	make definitions for Holland et al., 2013 mantle mineralogical model

As a general rule, however, it is always better not to exclude a priori any phase.

Include solution models (Y/N)?

n

Solid solutions are not considered in this case, because we are modelling reactions between end-member phases.

Enter calculation title:

ex2

(2) Doing the calculation (CONVEX)

Run CONVEX to make the calculation:

```
C:\PERPLEX\Perplex691>convex
```

Perple_X version 6.9.1, source updated January 3, 2022.

Copyright (C) 1986-2022 James A D Connolly <www.perplex.ethz.ch/copyright.html>.

Enter the project name (the name assigned in BUILD) [default = my_project]:

```
ex2
```

```
Reading problem definition from file: ex2.dat
```

```
Reading thermodynamic data from file: hp62ver.dat
```

```
Writing print output to file: ex2.plt
```

```
Writing plot output to file: ex2.plt
```

```
Reading solution models from file: not requested
```

```
Reading Perple_X options from: perplex_option.dat
```

```
Writing complete reaction list to: not requested
```

```
Writing Perple_X option summary to: not requested
```

Perple_X computational option settings for CONVEX:

```
Keyword:      Value:  Permitted values [default]:
```

Auto-refine options:

```
auto_refine   aut   [auto] manual off
```

```
replicate_threshold 0.1E-1 [1e-2]; static opt; <0 => no replica test
```

```
rep_dynamic_threshold 0.1E-2 [1d-3]; dynamic opt; <0 => no replica test
```

```
re-refine     F     [F] T
```

```
intermediate_savrpc F   [F] T
```

```
intermediate_savdyn F   [F] T
```

```
keep_all_rpcs  T    [T] F
```

Schreinemakers and Mixed-variable diagram options:

```
variance      1 /99 [1/99], >0; maximum true variance
```

```
increment     0.100/0.025 [0.1/0.025], default search/trace variable increment
```

```
efficiency    3    [3] >0, <6
```

```
reaction_format min  [min] full stoichiometry S+V everything
```

```
reaction_list off  [off] on
```

```
console_messages on  [on] off
```

```
short_print_file on  [on] off
```

Solution subdivision options:

initial_resolution:

```
exploratory stage 0.0625 0->1 [1/16], 0 => off
```

```
auto-refine stage 0.0208 0->1 [ ], 0 => off
```

```
stretch_factor 0.0020 >0 [2d-3]
```

```
non_linear_switch F    [F] T
```

```
subdivision_override off [off] lin str
```

```
hard_limits     off  [off] on
```

```
refine_endmembers F    [F] T
```

```
pc_perturbation 0.0050 [5d-3]
```

Thermodynamic options:

solvus_tolerance aut [aut] or 0->1; aut = automatic, 0 => p=c pseudocompounds, 1 => homogenize
 T_stop (K) 0.0 [0]
 T_melt (K) 873.0 [873]
 approx_alpha T [T] F
 Anderson-Gruneisen F [F] T
 speciation_precision 0.1E-4 [1d-5] <1; absolute
 speciation_max_it 100 [100]
 GFSM F [F] T GFSM/special_component toggle
 hybrid_EoS_H2O 4 [4] 0-2, 4-7
 hybrid_EoS_CO2 4 [4] 0-4, 7
 hybrid_EoS_CH4 0 [0] 0-1, 7
 aq_bad_results err [err] 101 102 103 ignore
 aq_lagged_speciation F [F] T
 aq_ion_H+ T [T] F => use OH-
 aq_oxide_components F [F] T
 aq_solvent_solvus T [T] F
 aq_vapor_epsilon 1.0 [1.]
 Input/Output options:
 pause_on_error T [T] F
 timing T [T] F
 auto_exclude T [T] F

To change these options see: www.perplex.ethz.ch/perplex_options.html

 Summary of make-definition entities:

fo8L q8L cenjh odi qjL dijl fojL foTL foHL qHL

 ** Starting auto_refine computational stage **

cycle	1	1	1
cycle	2	2	3
cycle	3	4	5
cycle	4	6	7

Initial number of divariant assemblages to be tested is: 7

Testing divariant assemblage 1, 6 assemblages remaining to be tested.

finished with equilibrium (1) br = per

Testing divariant assemblage 2, 6 assemblages remaining to be tested.

finished with equilibrium (2) q = trd

Testing divariant assemblage 3, 6 assemblages remaining to be tested.

finished with equilibrium (3) br atg = fo

finished with equilibrium (4) liz = br atg

Testing divariant assemblage 4, 9 assemblages remaining to be tested.

finished with equilibrium (5) tr = di q en

finished with equilibrium (6) di ta = tr

Testing divariant assemblage 5, 10 assemblages remaining to be tested.

finished with equilibrium (7) di atg = tr fo

Testing divariant assemblage 6, 12 assemblages remaining to be tested.

finished with equilibrium (8) ta = q anth

finished with equilibrium (9) ta = q en

finished with equilibrium (10) anth = q en

finished with equilibrium (11) ta en = anth

finished with equilibrium (12) ta fo = anth

finished with equilibrium (13) ta fo = en
 finished with equilibrium (14) anth fo = en
 finished with equilibrium (15) ta atg = en
 finished with equilibrium (16) atg = ta fo
 finished with equilibrium (17) atg = en fo
 Testing divariant assemblage 7, 12 assemblages remaining to be tested.
 finished with equilibrium (16) atg = ta fo
 Testing divariant assemblage 8, 12 assemblages remaining to be tested.
 Testing divariant assemblage 9, 12 assemblages remaining to be tested.
 Testing divariant assemblage 10, 12 assemblages remaining to be tested.
 Testing divariant assemblage 11, 11 assemblages remaining to be tested.
 Testing divariant assemblage 12, 11 assemblages remaining to be tested.
 Testing divariant assemblage 13, 11 assemblages remaining to be tested.
 Testing divariant assemblage 14, 11 assemblages remaining to be tested.
 Testing divariant assemblage 15, 11 assemblages remaining to be tested.
 Testing divariant assemblage 16, 12 assemblages remaining to be tested.
 Testing divariant assemblage 17, 11 assemblages remaining to be tested.
 finished with equilibrium (18) tr fo = di en
 Testing divariant assemblage 18, 14 assemblages remaining to be tested.
 Testing divariant assemblage 19, 15 assemblages remaining to be tested.
 Testing divariant assemblage 20, 15 assemblages remaining to be tested.
 Testing divariant assemblage 21, 16 assemblages remaining to be tested.
 Testing divariant assemblage 22, 15 assemblages remaining to be tested.
 Testing divariant assemblage 23, 14 assemblages remaining to be tested.
 Testing divariant assemblage 24, 14 assemblages remaining to be tested.
 Testing divariant assemblage 25, 13 assemblages remaining to be tested.
 Testing divariant assemblage 26, 12 assemblages remaining to be tested.
 Testing divariant assemblage 27, 12 assemblages remaining to be tested.
 Testing divariant assemblage 28, 11 assemblages remaining to be tested.
 Testing divariant assemblage 29, 10 assemblages remaining to be tested.
 Testing divariant assemblage 30, 10 assemblages remaining to be tested.
 Testing divariant assemblage 31, 9 assemblages remaining to be tested.
 Testing divariant assemblage 32, 8 assemblages remaining to be tested.
 Testing divariant assemblage 33, 8 assemblages remaining to be tested.
 Testing divariant assemblage 34, 7 assemblages remaining to be tested.
 Testing divariant assemblage 35, 6 assemblages remaining to be tested.
 Testing divariant assemblage 36, 5 assemblages remaining to be tested.
 Testing divariant assemblage 37, 5 assemblages remaining to be tested.
 Testing divariant assemblage 38, 4 assemblages remaining to be tested.
 Testing divariant assemblage 39, 3 assemblages remaining to be tested.
 Testing divariant assemblage 40, 4 assemblages remaining to be tested.
 Testing divariant assemblage 41, 5 assemblages remaining to be tested.
 Testing divariant assemblage 42, 6 assemblages remaining to be tested.
 Testing divariant assemblage 43, 5 assemblages remaining to be tested.
 Testing divariant assemblage 44, 5 assemblages remaining to be tested.
 Testing divariant assemblage 45, 4 assemblages remaining to be tested.
 warning ver066 Metastable assemblage into FLIPIT:
 tr atg en
 v = 20000.0 888.000 0.00000 0.00000 0.00000
 Testing divariant assemblage 46, 3 assemblages remaining to be tested.
 warning ver066 Metastable assemblage into FLIPIT:

```

tr   atg   fo
v = 20000.0  888.000  0.00000  0.00000  0.00000
Testing divariant assemblage  47,  2 assemblages remaining to be tested.
Testing divariant assemblage  48,  1 assemblages remaining to be tested.
Testing divariant assemblage  49,  0 assemblages remaining to be tested.
Testing divariant assemblage  50,  0 assemblages remaining to be tested.

```

(3a) Plotting the calculated phase diagram (PSVDRAW)

Run PSVDRAW to plot the calculated phase diagram:

```
C:\PERPLEX\Perplex691>psvdraw
```

Perple_X version 6.9.1, source updated January 3, 2022.

Copyright (C) 1986-2022 James A D Connolly <www.perplex.ethz.ch/copyright.html>.

Enter the project or plot file name [i.e., without the .plt suffix]:

```
ex2
```

Perple_X plot options are currently set as:

```

Keyword:      Value:  Permitted values [default]:
axis_label_scale  1.20  [1.2] (rel)
bounding_box :
    0  [0] x-min (pts)
    0  [0] y-min (pts)
    800 [800] x-length (pts)
    800 [800] y-length (pts)
field_fill      T  [T] F
field_label     T  [T] F
numeric_field_label F  [F] T, if T PSSECT writes list to *_assemblages.txt
replicate_label  0.250  0->1 [0.025]
field_label_scale  0.75  [0.72] (rel)
font            Helvetica
grid           F  [F] T
half_ticks     T  [T] F
line_width     1.00  0-99 [1.] (pts)
picture_transformation :
    0.180 [0.18] x-scale (rel)
    0.180 [0.18] y-scale (rel)
    130.  [0.18] x-translation (pts)
    220.  [0.18] y-translation (pts)
    0.00  [0.0] rotation (deg)
plot_aspect_ratio  1.000  [1.0] x_axis_length/y_axis_length
splines          T  [T] F
tenth_ticks     F  [F] T
text_scale      1.000  [1.] (rel)
plot_extra_data

```

To change these options edit or create the plot option file

See: www.perplex.ethz.ch/perplex_plot_options.html

(3b) Modifying the default plotting of the calculated phase diagram (PSVDRAW)

E.g. you want to modify the axes numbering (intervals on x axis = 100°C; intervals on y axis = 4 kbar) and to assign a numeric label (rather than a text label) to (most of) the reaction curves.

Run again PSVDRAW:

```
C:\PERPLEX\Perplex691>psvdraw
```

Perple_X version 6.9.1, source updated January 3, 2022.

Copyright (C) 1986-2022 James A D Connolly <www.perplex.ethz.ch/copyright.html>.

Enter the project or plot file name [i.e., without the .plt suffix]:

ex2

Perple_X plot options are currently set as:

Keyword:	Value:	Permitted values [default]:
axis_label_scale	1.20	[1.2] (rel)
bounding_box :		
	0	[0] x-min (pts)
	0	[0] y-min (pts)
	800	[800] x-length (pts)
	800	[800] y-length (pts)
field_fill	T	[T] F
field_label	T	[T] F
numeric_field_label	F	[F] T, if T PSSECT writes list to *_assemblages.txt
replicate_label	0.250	0->1 [0.025]
field_label_scale	0.75	[0.72] (rel)
font	Helvetica	
grid	F	[F] T
half_ticks	T	[T] F
line_width	1.00	0-99 [1.] (pts)
picture_transformation :		
	0.180	[0.18] x-scale (rel)
	0.180	[0.18] y-scale (rel)
	130.	[0.18] x-translation (pts)
	220.	[0.18] y-translation (pts)
	0.00	[0.0] rotation (deg)
plot_aspect_ratio	1.000	[1.0] x_axis_length/y_axis_length
splines	T	[T] F
tenth_ticks	F	[F] T
text_scale	1.000	[1.] (rel)
plot_extra_data		

To change these options edit or create the plot option file

See: www.perplex.ethz.ch/perplex_plot_options.html

PostScript will be written to file: ex2.ps

Modify the default plot (y/n)?

y

Modify drafting options (y/n)?

answer yes to modify:

- field labeling
- x-y plotting limits
- axes numbering

y

Modify x-y limits (y/n)?

Answer Y if you want to modify the T and/or P range of the diagram.

n

Restrict phase fields by variance (y/n)?

answer yes to:

- suppress pseudounivariant curves and/or pseudoinvariant points of a specified true variance.

n

Restrict phase fields by phase identities (y/n)?

answer yes to:

- show fields that contain a specific assemblage
- show fields that do not contain specified phases
- show fields that contain any of a set of specified phases

This question is only relevant for more complex calculations, involving solution models and therefore considering also pseudo-univariant curves (i.e. di-variant equilibria involving two pseudocompounds of the same phase as reactant and product). **See Ex. 7.**

n

Modify default equilibrium labeling (y/n)?

answer yes to:

- modify/suppress [pseudo-] univariant curve labels
- suppress [pseudo-] invariant point labels

y

Suppress curve labels (y/n)?

n

Change default labeling of curve segments (y/n)?

y

Suppress labels of pseudounivariant curves (y/n)?

y

Enter minimum fraction of the axes length that a curve must be to receive a text label (0-1):

1 means that a text label will be assigned to those curves that are longer than the axes length.

1

Enter minimum fraction of the axes length that a curve must be to receive a numeric label (0-1.000):

0 means that a numeric label will be assigned to all those curves that are shorter than the axes length.

0

Suppress point labels (y/n)?

n

Modify default axes numbering (y/n)?

y

Enter the starting value and interval for major tick marks on the X-axis (current values are: 473. 160.)

Enter the new values:

473

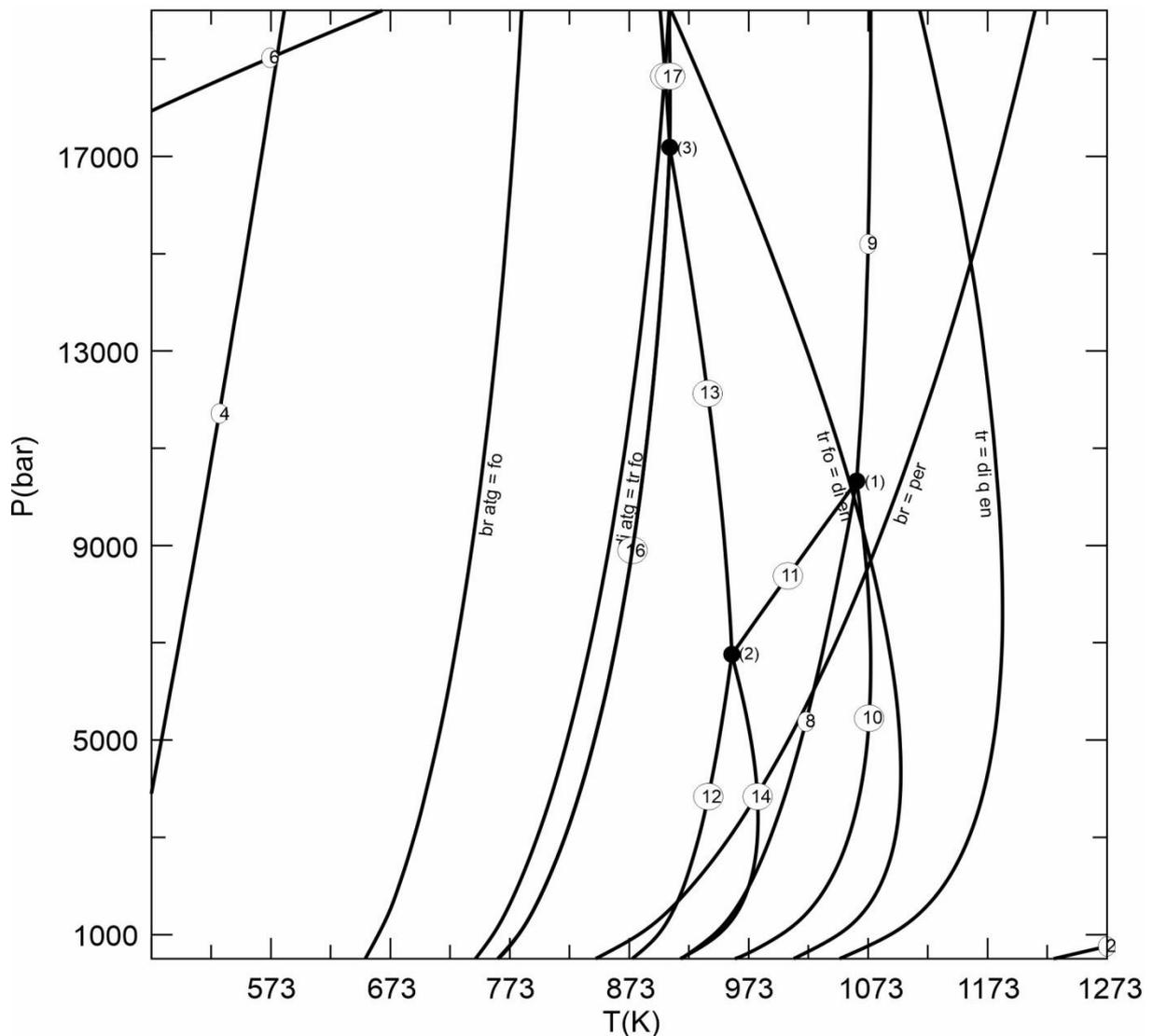
100

Enter the starting value and interval for major tick marks on the Y-axis (current values are: 500. 0.390E+04)

Enter the new values:

1000

4000



Equilibria corresponding to each reaction number are explained in the ex2.prn file.

Ex 3

n

Specify computational mode:

- 1 - Convex-Hull minimization
- 2 - Constrained minimization on a 2d grid [default]
- 3 - Constrained minimization on a 1d grid
- 4 - Output pseudocompound data
- 5 - 1-d Phase fractionation
- 6 - 0-d Infiltration-reaction-fractionation
- 7 - 2-d Phase fractionation (FRAC2D and TITRATE reactive transport models)

Use Convex-Hull minimization for Schreinemakers projections or phase diagrams with > 2 independent variables. Use constrained minimization for phase diagrams or phase diagram sections with < 3 independent variables.

1

Use option 1 (Convex-Hull minimization) for PROJECTIONS (Schreinemakers-type diagrams) or CHEMOGRAPHIES (composition diagrams; phase diagrams with > 2 independent variables). Use options 2 or 3 (Constrained minimization on a 2d grid/1d grid) for PSEUDOSECTIONS (phase diagrams or phase diagram sections with < 3 independent variables).

Calculations with a saturated fluid (Y/N)?

y

Select the independent saturated fluid components:

H2O CO2

Enter names, 1 per line, press <enter> to finish:

For C-O-H fluids it is only necessary to select volatile species present in the solids of interest. If the species listed here are H2O and CO2, then to constrain O2 chemical potential to be consistent with C-O-H fluid speciation treat O2 as a saturated component. Refer to the Perple_X Tutorial for details.

H2O

Calculations with saturated components (Y/N)?

n

Use chemical potentials, activities or fugacities as independent variables (Y/N)?

n

Select thermodynamic components from the set:

Na2O MgO Al2O3 SiO2 K2O CaO TiO2 MnO FeO NiO ZrO2 Cl2 O2 CO2 CuO Cr2O3 S2 F2 N2 ZnO

Enter names, 1 per line, press <enter> to finish:

CaO

MgO

SiO2

The order (1st, 2nd, 3rd) influences how the three components are plotted in the chemographies: first = bottom left, second = bottom right, third = top.

Because the thermodynamic data file identifies: H2O as special components, you will be prompted next for the EoS to be used for the corresponding components and mixtures thereof. To override this behavior, e.g., to use a generic hybrid fluid EoS, delete the special_component section from the thermodynamic data file header.

NOTE: the EoS choice specified here will override the EoS choice specified by the hybrid_EoS option, to override this behavior delete the special_component section from the the thermodynamic data file header.

Select fluid equation of state:

- 0 - X(CO2) H2O-CO2 Modified Redlich-Kwong (MRK) DeSantis et al 74
- 1 - X(CO2) H2O-CO2 HSMRK Kerrick & Jacobs 81
- 2 - X(CO2) H2O-CO2 MRK hybrid-EoS*
- 5 - X(CO2) H2O-CO2 CORK Holland & Powell 91, 98
- 8 - f(O2/CO2) C-buffered COH MRK hybrid-EoS*
- 10 - X(O) C-buffered COH MRK hybrid-EoS Connolly & Cesare 93*
- 12 - X(O)-f(S2) C-buffered COHS MRK hybrid-EoS Connolly & Cesare 93*
- 13 - X(H2) H2O-H2 MRK hybrid-EoS*
- 14 - X(CO2) H2O-CO2 Pitzer & Sterner 94; Holland & Powell mixing 03
- 15 - X(H2) H2O-H2 low T MRK hybrid-EoS*
- 16 - X(O) H-O MRK hybrid-EoS*
- 17 - X(O)-f(S2) H-O-S MRK hybrid-EoS*
- 19 - X(O)-X(S) C-buffered COHS MRK hybrid-EoS Connolly & Cesare 93*
- 20 - X(O)-X(C) COHS MRK hybrid-EoS Connolly & Cesare 93*
- 24 - f(O2/CO2)-N/C C-buffered COHN MRK hybrid-EoS*
- 25 - X(CO2)-X(NaCl) H2O-CO2-NaCl Aranovich et al 10
- 26 - X(O) O-Si MRK Connolly 16
- 27 - X(O)-X(C) C-O-H MRK hybrid-EoS*

*Hybrid EoS use the following pure species EoS, to change these associations modify the hybrid_EoS keywords in the perplex_option file:

- H2O - PSEoS Pitzer & Sterner 1994
- CO2 - PSEoS Pitzer & Sterner 1994
- CH4 - MRK DeSantis et al 1974

5

The data base has P(bar) and T(K) as default independent potentials.

Make one dependent on the other, e.g., as along a geothermal gradient (y/n)?

n

Specify number of independent potential variables:

- 0 - Composition diagram [default]
- 1 - Mixed-variable diagram
- 2 - Sections and Schreinemakers-type diagrams

0

Output a print file (Y/N)?

y

Exclude pure and/or endmember phases (Y/N)?

y

Do you want to be prompted for phases (Y/N)?

n

Enter names, 1 per line, press <enter> to finish:

Same as in Ex. 2

rnk | rankinite Ca3Si2O7

lrn | larnite Ca₂SiO₄
 cstn | "Si-titanite" CaSi₂O₅ (one Si replaces Ti)
 wo | wollastonite CaSiO₃
 pswo | pseudo-wollastonite CaSiO₃
 wal | wollastonite CaSiO₃
 ak | akermanite Ca₂MgSi₂O₇
 merw | merwinite Ca₃MgSi₂O₈
 mont | monticellite CaMgSiO₄
 chum | clinohumite Mg₉Si₄O₁₆(OH)₂
 cen | clinoenstatite Mg₂Si₂O₆
 cumm | cummingtonite Mg₇Si₈O₂₂(OH)₂
 cumm_dqf | cummingtonite for Diener et al. (2007) cAmph model
 woL | wollastonite LIQUID
 limL | lime LIQUID
 mcpv | make definitions for Holland et al., 2013 mantle mineralogical model
 cmpv | make definitions for Holland et al., 2013 mantle mineralogical model
 cpv | make definitions for Holland et al., 2013 mantle mineralogical model

Include solution models (Y/N)?

n

Enter calculation title:

ex3

*Although only one component is specified for the fluid phase, its equation of state permits use of its compositional variable: Y(CO₂) .

Specify values for: P(bar) T(K) Y(CO₂). For calculation 1, enter zeros to finish.

Here you must specify at which P-T-XCO₂ conditions you would like to calculate the chemographies. Having included only H₂O as saturated fluid component, XCO₂ is always 0.

Point A:

3000

573

0

Specify values for: P(bar) T(K) Y(CO₂). For calculation 2, enter zeros to finish.

Point B:

5000

733

0

Specify values for: P(bar) T(K) Y(CO₂). For calculation 3, enter zeros to finish.

Point C:

7000

843

0

Specify values for: P(bar) T(K) Y(CO₂). For calculation 4, enter zeros to finish.

Point D:

8000
893
0

Specify values for: P(bar) T(K) Y(CO₂). For calculation 5, enter zeros to finish.

Point E:

9000
973
0

Specify values for: P(bar) T(K) Y(CO₂). For calculation 6, enter zeros to finish.

Point F:

11000
1093
0

Specify values for: P(bar) T(K) Y(CO₂). For calculation 7, enter zeros to finish.

Point G:

4000
843
0

Specify values for: P(bar) T(K) Y(CO₂). For calculation 8, enter zeros to finish.

Point H:

5000
963
0

Specify values for: P(bar) T(K) Y(CO₂). For calculation 9, enter zeros to finish.

Point I:

6000
1073
0

Specify values for: P(bar) T(K) Y(CO₂) For calculation 10, enter zeros to finish.

0
0
0

(2) Doing the calculation (CONVEX)

Run CONVEX to make the calculation:

```
C:\PERPLEX\Perplex691>convex
```

Perple_X version 6.9.1, source updated January 3, 2022.

Copyright (C) 1986-2022 James A D Connolly <www.perplex.ethz.ch/copyright.html>.

Enter the project name (the name assigned in BUILD) [default = my_project]:

ex3

Reading problem definition from file: ex3.dat
Reading thermodynamic data from file: hp62ver.dat
Writing print output to file: ex3.plt
Writing plot output to file: ex3.plt
Reading solution models from file: not requested
Reading Perple_X options from: perplex_option.dat
Writing Perple_X option summary to: not requested

Perple_X computational option settings for CONVEX:

Keyword: Value: Permitted values [default]:

Auto-refine options:

auto_refine aut [auto] manual off
replicate_threshold 0.1E-1 [1e-2]; static opt; <0 => no replica test
rep_dynamic_threshold 0.1E-2 [1d-3]; dynamic opt; <0 => no replica test
re-refine F [F] T
intermediate_savrpc F [F] T
intermediate_savdyn F [F] T
keep_all_rpcs T [T] F

Solution subdivision options:

initial_resolution:
exploratory stage 0.0625 0->1 [1/16], 0 => off
auto-refine stage 0.0063 0->1 [], 0 => off
stretch_factor 0.0020 >0 [2d-3]
non_linear_switch F [F] T
subdivision_override off [off] lin str
hard_limits off [off] on
refine_endmembers F [F] T
pc_perturbation 0.0050 [5d-3]

Thermodynamic options:

solvus_tolerance aut [aut] or 0->1; aut = automatic, 0 => p=c pseudocompounds, 1 => homogenize
T_stop (K) 0.0 [0]
T_melt (K) 873.0 [873]
approx_alpha T [T] F
Anderson-Gruneisen F [F] T
speciation_precision 0.1E-4 [1d-5] <1; absolute
speciation_max_it 100 [100]
GFSM F [F] T GFSM/special_component toggle
hybrid_EoS_H2O 4 [4] 0-2, 4-7
hybrid_EoS_CO2 4 [4] 0-4, 7
hybrid_EoS_CH4 0 [0] 0-1, 7
aq_bad_results err [err] 101 102 103 ignore
aq_lagged_speciation F [F] T
aq_ion_H+ T [T] F => use OH-
aq_oxide_components F [F] T
aq_solvent_solvus T [T] F
aq_vapor_epsilon 1.0 [1.]

Input/Output options:

pause_on_error T [T] F
timing T [T] F
auto_exclude T [T] F

To change these options see: www.perplex.ethz.ch/perplex_options.html

Summary of make-definition entities:

fo8L q8L cenjh odi qjL dijl
fojL foTL foHL qHL

** Starting auto_refine computational stage **

Computing the compositional phase relations at condition 1

cycle 1 1 1
cycle 2 2 3
cycle 3 4 5
cycle 4 6 7

Computing the compositional phase relations at condition 2

cycle 1 1 1
cycle 2 2 3
cycle 3 4 5
cycle 4 6 7
cycle 5 8 8

Computing the compositional phase relations at condition 3

cycle 1 1 1
cycle 2 2 3
cycle 3 4 5
cycle 4 6 7
cycle 5 8 8

Computing the compositional phase relations at condition 4

cycle 1 1 1
cycle 2 2 3
cycle 3 4 5
cycle 4 6 7

Computing the compositional phase relations at condition 5

cycle 1 1 1
cycle 2 2 3
cycle 3 4 5
cycle 4 6 7
cycle 5 8 8

Computing the compositional phase relations at condition 6

cycle 1 1 1
cycle 2 2 3
cycle 3 4 5
cycle 4 6 7

Computing the compositional phase relations at condition 7

cycle 1 1 1
cycle 2 2 3
cycle 3 4 5
cycle 4 6 7

Computing the compositional phase relations at condition 8

cycle 1 1 1
cycle 2 2 3

```
cycle 3 4 5
cycle 4 6 7
cycle 5 8 8
```

Computing the compositional phase relations at condition 9

```
cycle 1 1 1
cycle 2 2 3
cycle 3 4 5
cycle 4 6 7
cycle 5 8 8
```

(3) Plotting the calculated phase diagram (PSVDRAW)

Run PSVDRAW to plot the calculated chemographies:

```
C:\PERPLEX\Perplex691>psvdraw
```

Perple_X version 6.9.1, source updated January 3, 2022.

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Enter the project or plot file name [i.e., without the .plt suffix]:

ex3

Perple_X plot options are currently set as:

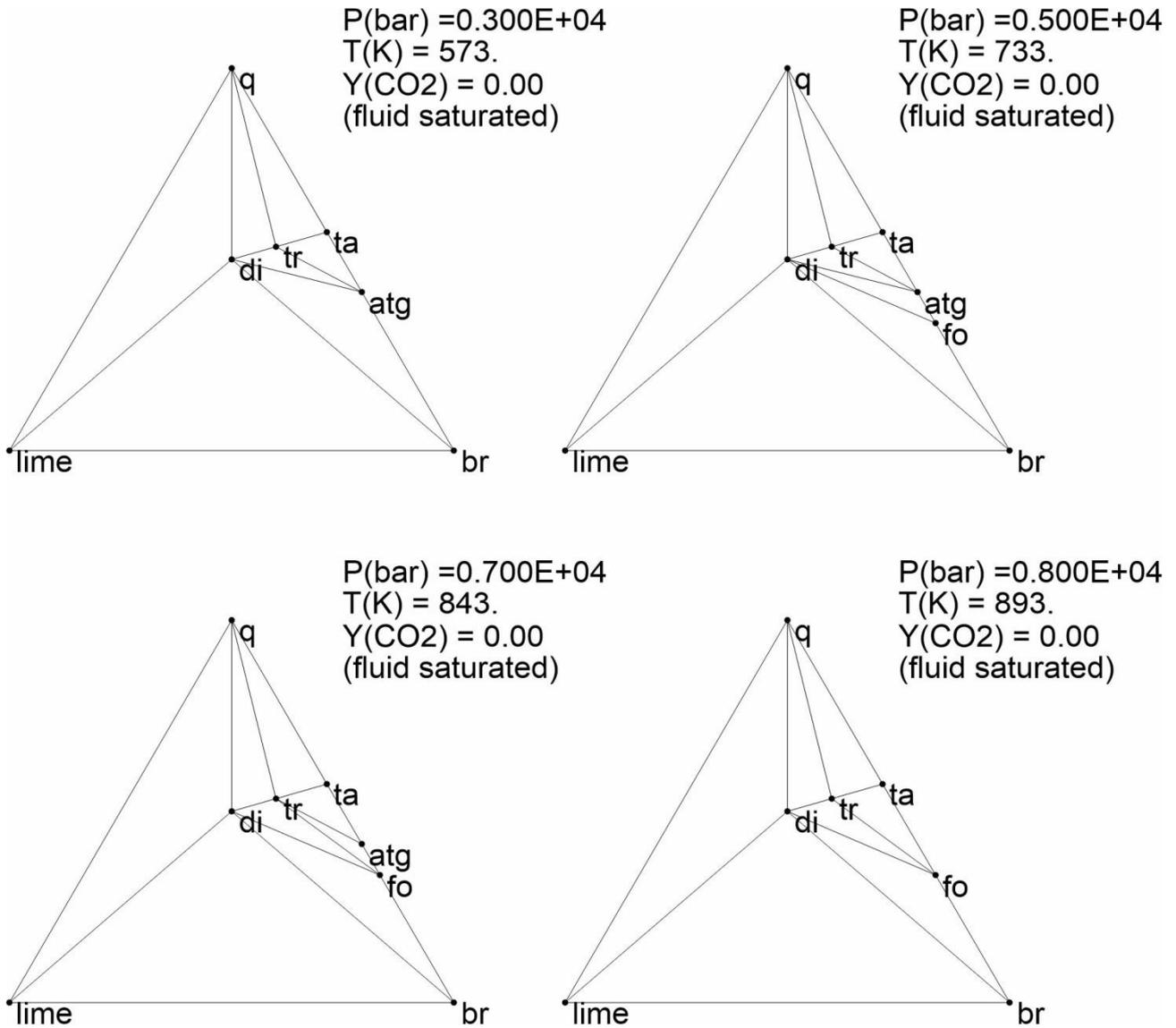
```
Keyword:      Value:  Permitted values [default]:
axis_label_scale  1.20  [1.2] (rel)
bounding_box :
    0  [0] x-min (pts)
    0  [0] y-min (pts)
    800 [800] x-length (pts)
    800 [800] y-length (pts)
field_fill      T  [T] F
field_label     T  [T] F
numeric_field_label F  [F] T, if T PSSECT writes list to *_assemblages.txt
replicate_label 0.250 0->1 [0.025]
field_label_scale 0.75  [0.72] (rel)
font            Helvetica
grid            F  [F] T
half_ticks      T  [T] F
line_width      1.00  0-99 [1.] (pts)
picture_transformation :
    0.180 [0.18] x-scale (rel)
    0.180 [0.18] y-scale (rel)
    130.  [0.18] x-translation (pts)
    220.  [0.18] y-translation (pts)
    0.00  [0.0] rotation (deg)
plot_aspect_ratio 1.000 [1.0] x_axis_length/y_axis_length
splines          T  [T] F
tenth_ticks      F  [F] T
text_scale       1.000 [1.] (rel)
plot_extra_data
```

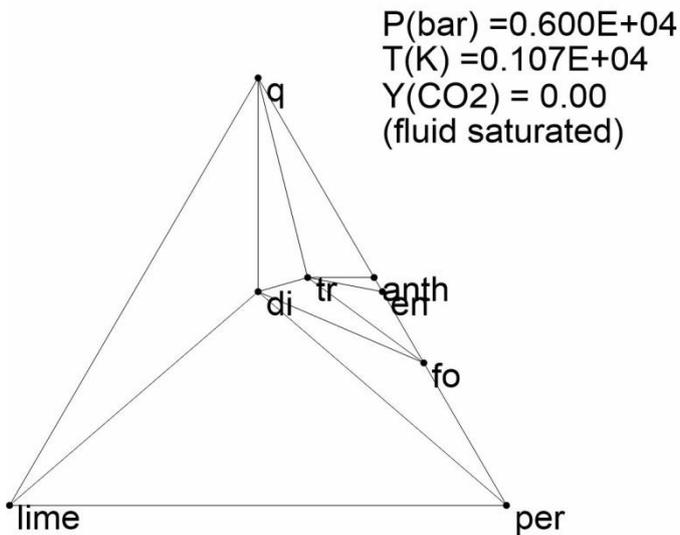
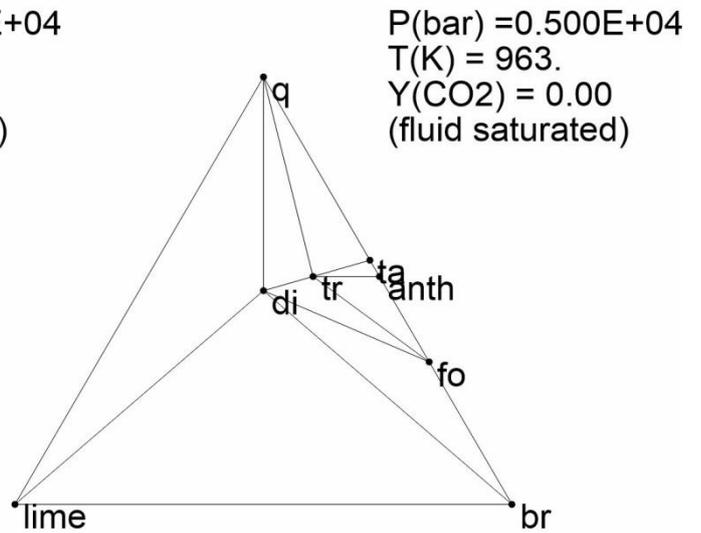
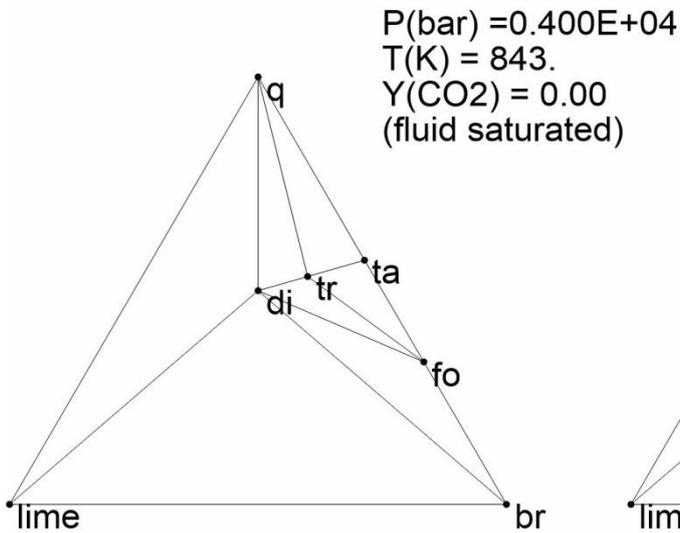
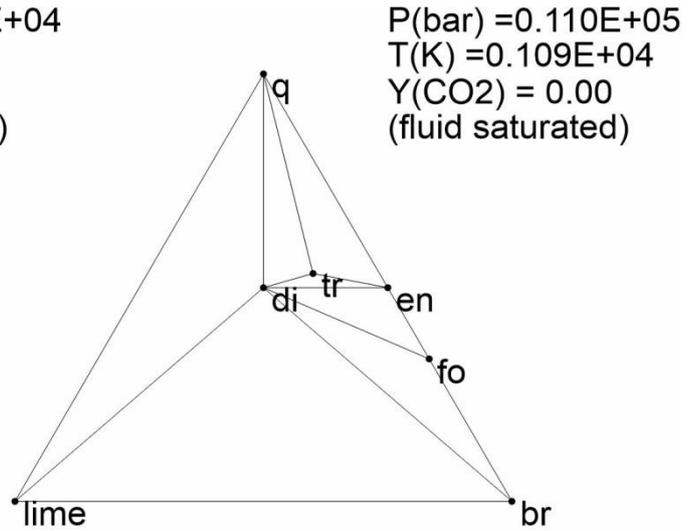
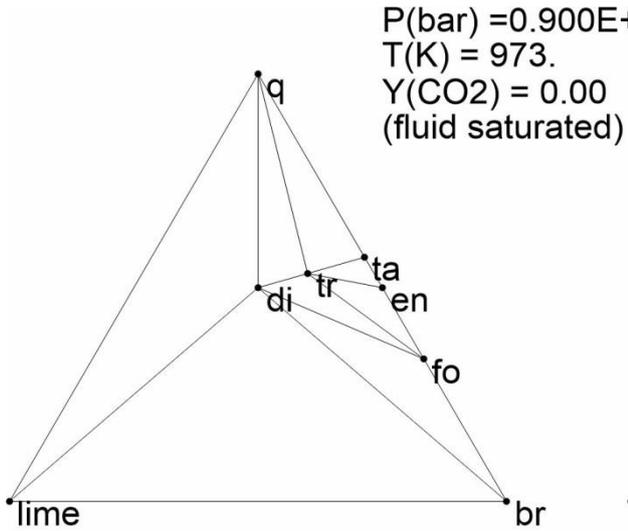
To change these options edit or create the plot option file
See: www.perplex.ethz.ch/perplex_plot_options.html

PostScript will be written to file: ex3.ps

Modify the default plot (y/n)?

N

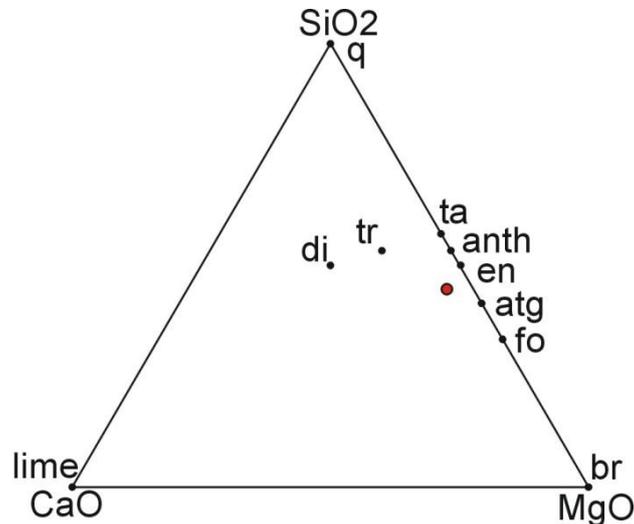




Ex 4

Ex. 4 – P-T pseudosection for the CMSH system (no solid solutions)

This exercise explains how to calculate a very simple pseudosection, not involving solid solutions, for a generic ultramafic composition (MgO=50, SiO₂=45, CaO=5 mol%; red dot in the figure below).



Combined with Ex. 2 and Ex. 3, this exercise is useful to understand the difference between P-T projections and P-T pseudosections.

(1) Definition of the problem (BUILD)

```
C:\PERPLEX\Perplex691>build
```

Perple_X version 6.9.1, source updated January 3, 2022.

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NO is the default (blank) answer to all Y/N prompts

Enter a name for this project (the name will be used as the root for all output file names) [default = my_project]:

ex4

The problem definition file will be named: ex4.dat

Enter thermodynamic data file name [default = hp02ver.dat]:

hp62ver.dat

Enter the computational option file name [default = perplex_option.dat]:

See: www.perplex.ethz.ch/perplex_options.html

[enter]

Reading Perple_X options from: perplex_option.dat

The current data base components are:

Na2O MgO Al2O3 SiO2 K2O CaO TiO2 MnO FeO NiO ZrO2 Cl2 O2 H2O CO2 CuO Cr2O3 S2 F2 N2 ZnO
Transform them (Y/N)?

n

Specify computational mode:

- 1 - Convex-Hull minimization
- 2 - Constrained minimization on a 2d grid [default]
- 3 - Constrained minimization on a 1d grid
- 4 - Output pseudocompound data
- 5 - 1-d Phase fractionation
- 6 - 0-d Infiltration-reaction-fractionation
- 7 - 2-d Phase fractionation (FRAC2D and TITRATE reactive transport models)

Use Convex-Hull minimization for Schreinemakers projections or phase diagrams with > 2 independent variables. Use constrained minimization for phase diagrams or phase diagram sections with < 3 independent variables.

2

Use option 1 (Convex-Hull minimization) for PROJECTIONS (Schreinemakers-type diagrams) or CHEMOGRAPHIES (composition diagrams; phase diagrams with > 2 independent variables). Use options 2 or 3 (Constrained minimization on a 2d grid/1d grid) for PSEUDOSECTIONS (phase diagrams or phase diagram sections with < 3 independent variables).

Calculations with a saturated fluid (Y/N)?

y

Select the independent saturated fluid components:

H2O CO2

Enter names, 1 per line, press <enter> to finish:

For C-O-H fluids it is only necessary to select volatile species present in the solids of interest. If the species listed here are H2O and CO2, then to constrain O2 chemical potential to be consistent with C-O-H fluid speciation treat O2 as a saturated component. Refer to the Perple_X Tutorial for details.

H2O

Calculations with saturated components (Y/N)?

n

Use chemical potentials, activities or fugacities as independent variables (Y/N)?

n

Select thermodynamic components from the set:

Na2O MgO Al2O3 SiO2 K2O CaO TiO2 MnO FeO NiO ZrO2 Cl2 O2 CO2 CuO Cr2O3 S2 F2 N2

Enter names, 1 per line, press <enter> to finish:

MgO

SiO2

CaO

Because the thermodynamic data file identifies: H2O as special components, you will be prompted next for the EoS to be used for the corresponding components and mixtures thereof. To override this behavior, e.g., to use a generic hybrid fluid EoS, delete the special_component section from the thermodynamic data file header.

NOTE: the EoS choice specified here will override the EoS choice specified by the hybrid_EoS option, to override this behavior delete the special_component section from the the thermodynamic data file header.

Select fluid equation of state:

- 0 - X(CO2) H2O-CO2 Modified Redlich-Kwong (MRK) DeSantis et al 74
- 1 - X(CO2) H2O-CO2 HSMRK Kerrick & Jacobs 81
- 2 - X(CO2) H2O-CO2 MRK hybrid-EoS*
- 5 - X(CO2) H2O-CO2 CORK Holland & Powell 91, 98
- 8 - f(O2/CO2) C-buffered COH MRK hybrid-EoS*
- 10 - X(O) C-buffered COH MRK hybrid-EoS Connolly & Cesare 93*
- 12 - X(O)-f(S2) C-buffered COHS MRK hybrid-EoS Connolly & Cesare 93*
- 13 - X(H2) H2O-H2 MRK hybrid-EoS*
- 14 - X(CO2) H2O-CO2 Pitzer & Sterner 94; Holland & Powell mixing 03
- 15 - X(H2) H2O-H2 low T MRK hybrid-EoS*
- 16 - X(O) H-O MRK hybrid-EoS*
- 17 - X(O)-f(S2) H-O-S MRK hybrid-EoS*
- 19 - X(O)-X(S) C-buffered COHS MRK hybrid-EoS Connolly & Cesare 93*
- 20 - X(O)-X(C) COHS MRK hybrid-EoS Connolly & Cesare 93*
- 24 - f(O2/CO2)-N/C C-buffered COHN MRK hybrid-EoS*
- 25 - X(CO2)-X(NaCl) H2O-CO2-NaCl Aranovich et al 10
- 26 - X(O) O-Si MRK Connolly 16
- 27 - X(O)-X(C) C-O-H MRK hybrid-EoS*

*Hybrid EoS use the following pure species EoS, to change these associations modify the hybrid_EoS keywords in the perplex_option file:

- H2O - PSEoS Pitzer & Sterner 1994
- CO2 - PSEoS Pitzer & Sterner 1994
- CH4 - MRK DeSantis et al 1974

5

The data base has P(bar) and T(K) as default independent potentials.

Make one dependent on the other, e.g., as along a geothermal gradient (y/n)?

n

Select x-axis variable:

- 1 - P(bar)
- 2 - T(K)
- 3 - Y(CO2)
- 4 - Composition X_C1* (user defined)

*Although only one component is specified for the Y(CO2) phase, its equation of state permits use of its compositional variable:

*X_C1 can not be selected as the y-axis variable

2

Enter minimum and maximum values, respectively, for: T(K)

473

1273

Select y-axis variable:

2 - P(bar)

3 - Y(CO2)

2

Enter minimum and maximum values, respectively, for: P(bar)

500

20000

Specify sectioning value for: Y(CO2)

0

For gridded minimization, grid resolution is determined by the number of levels (grid_levels) and the resolution at the lowest level in the X- and Y-directions (x_nodes and y_nodes) these parameters are currently set for the exploratory and autorefine cycles as follows:

stage	grid_levels	xnodes	ynodes	effective resolution
-------	-------------	--------	--------	----------------------

exploratory	1	10	10	10 x 10 nodes
-------------	---	----	----	---------------

auto-refine	4	40	40	313 x 313 nodes
-------------	---	----	----	-----------------

To change these options edit or create the file perplex_option.dat

See: www.perplex.ethz.ch/perplex_options.html#grid_parameters

Specify component amounts by mass (Y/N)?

n

[Here you can specify the bulk composition of your sample either in wt% \(by mass\) or in mol%. In this example, that refers to a generic ultramafic rock rather than to a real sample, I have chosen mol% because it is easier to visualize a mol% composition on the chemographies.](#)

The amounts you enter next need not be normalized; regardless of units, they define the molar amount of the system

Enter the molar amounts of the components:

MgO SiO2 CaO

for the bulk composition of interest:

50

45

5

Output a print file (Y/N)?

y

Exclude pure and/or endmember phases (Y/N)?

y

Do you want to be prompted for phases (Y/N)?

n

Enter names, 1 per line, press <enter> to finish:

[Same as in Ex. 2 and Ex. 3.](#)

rnk | rankinite Ca3Si2O7

lrn | larnite Ca₂SiO₄
 cstn | "Si-titanite" CaSi₂O₅ (one Si replaces Ti)
 wo | wollastonite CaSiO₃
 pswo | pseudo-wollastonite CaSiO₃
 wal | wollastonite CaSiO₃
 ak | akermanite Ca₂MgSi₂O₇
 merw | merwinite Ca₃MgSi₂O₈
 mont | monticellite CaMgSiO₄
 chum | clinohumite Mg₉Si₄O₁₆(OH)₂
 cen | clinoenstatite Mg₂Si₂O₆
 cumm | cummingtonite Mg₇Si₈O₂₂(OH)₂
 cumm_dqf | cummingtonite for Diener et al. (2007) cAmph model
 woL | wollastonite LIQUID
 limL | lime LIQUID
 mcpv | make definitions for Holland et al., 2013 mantle mineralogical model
 cmpv | make definitions for Holland et al., 2013 mantle mineralogical model
 cpv | make definitions for Holland et al., 2013 mantle mineralogical model

Include solution models (Y/N)?

n

Enter calculation title:

ex4

(2) Doing the calculation (VERTEX)

Run VERTEX to make the calculation:

C:\PERPLEX\Perplex691>vertex

Perple_X version 6.9.1, source updated January 3, 2022.

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Enter the project name (the name assigned in BUILD) [default = my_project]:

ex4

Reading problem definition from file: ex4.dat

Reading thermodynamic data from file: hp62ver.dat

Writing print output to file: ex4.plt

Writing plot output to file: ex4.plt

Writing phase assemblage data to file: ex4.blk

Reading solution models from file: not requested

Reading Perple_X options from: perplex_option.dat

Writing seismic data options to: ex4_seismic_data.txt

Writing Perple_X option summary to: not requested

Perple_X computational option settings for VERTEX:

Keyword: Value: Permitted values [default]:

Auto-refine options:

auto_refine aut [auto] manual off
 replicate_threshold 0.1E-1 [1e-2]; static opt; <0 => no replica test
 rep_dynamic_threshold 0.1E-2 [1d-3]; dynamic opt; <0 => no replica test
 re-refine F [F] T
 intermediate_savrpc F [F] T
 intermediate_savdyn F [F] T
 keep_all_rpcs T [T] F

Free energy minimization options:

MINFRC_diff_increment 0.1E-6 [1e-7] 1e-3 => 1e-9
 MINFXC_solver 0 [0] >= 0 - speci2, -1 - MINFXC
 optimization_max_it 40 [40] >1
 optimization_precision 0.1E-3 [1e-4], 1e-1 => 1e-6, absolute
 order_check F [F] T
 refinement_points 5 [auto] 1->14
 refinement_switch F [T] F
 scatter-points T [T] F
 scatter-increment 0.1E-1 [1e-2] 1e-2 => 1e-7
 solvus_tolerance_ll aut [0.2] 0->1
 zero_mode 0.1E-5 [1e-6] 0->1; < 0 => off

2D grid options:

x_nodes 10 / 40 [10/40] >0, <2048; effective x-resolution 10 / 313 nodes
 y_nodes 10 / 40 [10/40] >0, <2048; effective y-resolution 10 / 313 nodes
 grid_levels 1 / 4 [1/4] >0, <10
 linear_model on [on] off

Solution subdivision options:

initial_resolution: 0.2500 [1/4] 0->1; 0 => off
 stretch_factor 0.0020 [2d-3] >0
 non_linear_switch F [F] T
 subdivision_override off [lin] off str
 refine_endmembers F [F] T

Thermodynamic options:

solvus_tolerance aut [aut] or 0->1; aut = automatic, 0 => p=c pseudocompounds, 1 => homogenize
 T_stop (K) 0.0 [0]
 T_melt (K) 873.0 [873]
 approx_alpha T [T] F
 Anderson-Gruneisen F [F] T
 speciation_precision 0.1E-4 [1d-5] <1; absolute
 speciation_max_it 100 [100]
 GFSM F [F] T GFSM/special_component toggle
 hybrid_EoS_H2O 4 [4] 0-2, 4-7
 hybrid_EoS_CO2 4 [4] 0-4, 7
 hybrid_EoS_CH4 0 [0] 0-1, 7
 aq_bad_results err [err] 101 102 103 ignore
 aq_lagged_speciation F [F] T
 aq_ion_H+ T [T] F => use OH-
 aq_oxide_components F [F] T
 aq_solvent_solvus T [T] F
 aq_vapor_epsilon 1.0 [1.]

Input/Output options:

pause_on_error T [T] F
 timing T [T] F

auto_exclude T [T] F
logarithmic_p F [F] T
bad_number NaN [NaN]
interim_results aut [auto] off manual

Information file output options:

option_list_files F [F] T; echo computational options
pseudocompound_file F [F] T; echo static pseudocompound compositions
auto_refine_file F [T] F; echo auto-refine compositions
seismic_data_file T [F] T; echo seismic wavespeed options

To change these options see: www.perplex.ethz.ch/perplex_options.html

Summary of make-definition entities:

fo8L q8L cenjh odi qjL dijl
fojL foTL foHL qHL

warning ver099 no data for aqueous species, aq_output and aq_lagged_speciation disabled.

** Starting exploratory computational stage **

2.5% done with low level grid.
5.0% done with low level grid.
7.5% done with low level grid.
10.0% done with low level grid.
12.5% done with low level grid.
15.0% done with low level grid.
17.5% done with low level grid.
20.0% done with low level grid.
22.5% done with low level grid.
25.0% done with low level grid.
27.5% done with low level grid.
30.0% done with low level grid.
32.5% done with low level grid.
35.0% done with low level grid.
37.5% done with low level grid.
40.0% done with low level grid.
42.5% done with low level grid.
45.0% done with low level grid.
47.5% done with low level grid.
50.0% done with low level grid.
52.5% done with low level grid.
55.0% done with low level grid.
57.5% done with low level grid.
60.0% done with low level grid.
62.5% done with low level grid.
65.0% done with low level grid.
67.5% done with low level grid.
70.0% done with low level grid.
72.5% done with low level grid.
75.0% done with low level grid.
77.5% done with low level grid.
80.0% done with low level grid.
82.5% done with low level grid.

85.0% done with low level grid.
87.5% done with low level grid.
90.0% done with low level grid.
92.5% done with low level grid.
95.0% done with low level grid.
97.5% done with low level grid.
100.0% done with low level grid.

Beginning grid refinement stage.

197 grid cells to be refined at grid level 2
refinement at level 2 involved 429 minimizations
2029 minimizations required of the theoretical limit of 6241
380 grid cells to be refined at grid level 3
...working (73 minimizations done)
...working (576 minimizations done)
refinement at level 3 involved 745 minimizations
2774 minimizations required of the theoretical limit of 24649
719 grid cells to be refined at grid level 4
...working (333 minimizations done)
...working (834 minimizations done)
...working (1336 minimizations done)
refinement at level 4 involved 1363 minimizations
4137 minimizations required of the theoretical limit of 98596

Exploratory stage generated:

Total number of compositions: 0

**** Starting auto-refine computational stage ****

2.5% done with low level grid.
5.0% done with low level grid.
7.5% done with low level grid.
10.0% done with low level grid.
12.5% done with low level grid.
15.0% done with low level grid.
17.5% done with low level grid.
20.0% done with low level grid.
22.5% done with low level grid.
25.0% done with low level grid.
27.5% done with low level grid.
30.0% done with low level grid.
32.5% done with low level grid.
35.0% done with low level grid.
37.5% done with low level grid.
40.0% done with low level grid.
42.5% done with low level grid.
45.0% done with low level grid.
47.5% done with low level grid.
50.0% done with low level grid.
52.5% done with low level grid.
55.0% done with low level grid.
57.5% done with low level grid.

60.0% done with low level grid.
 62.5% done with low level grid.
 65.0% done with low level grid.
 67.5% done with low level grid.
 70.0% done with low level grid.
 72.5% done with low level grid.
 75.0% done with low level grid.
 77.5% done with low level grid.
 80.0% done with low level grid.
 82.5% done with low level grid.
 85.0% done with low level grid.
 87.5% done with low level grid.
 90.0% done with low level grid.
 92.5% done with low level grid.
 95.0% done with low level grid.
 97.5% done with low level grid.
 100.0% done with low level grid.

Beginning grid refinement stage.

197 grid cells to be refined at grid level 2
 refinement at level 2 involved 429 minimizations
 2029 minimizations required of the theoretical limit of 6241
 380 grid cells to be refined at grid level 3
 ...working (73 minimizations done)
 ...working (576 minimizations done)
 refinement at level 3 involved 745 minimizations
 2774 minimizations required of the theoretical limit of 24649
 719 grid cells to be refined at grid level 4
 ...working (333 minimizations done)
 ...working (834 minimizations done)
 ...working (1336 minimizations done)
 refinement at level 4 involved 1363 minimizations
 4137 minimizations required of the theoretical limit of 98596

Timing	min.	% of total
Static G calculation	0.26042E-03	2.9
Dynamic G calculation	0.0000	0.0
Static LP	0.0000	0.0
Dynamic LP	0.0000	0.0
Successive QP	0.0000	0.0
Total of above	0.26042E-03	2.9
Total elapsed time	0.91146E-02	100.0

End of job: ex4

(3) Plotting the calculated phase diagram (PSSECT)

Run PSSECT to plot the calculated pseudosection:

```
C:\PERPLEX\Perplex691>pssect
```

Perple_X version 6.9.1, source updated January 3, 2022.

Copyright (C) 1986-2022 James A D Connolly <www.perplex.ethz.ch/copyright.html>.

Enter the project name (the name assigned in BUILD) [default = my_project]:

```
ex4
```

Reading Perple_X options from: perplex_option.dat

Perple_X plot options are currently set as:

```
Keyword:      Value:  Permitted values [default]:
axis_label_scale  1.20  [1.2] (rel)
bounding_box :
      0  [0] x-min (pts)
      0  [0] y-min (pts)
      800 [800] x-length (pts)
      800 [800] y-length (pts)
field_fill      T  [T] F
field_label     T  [T] F
numeric_field_label  F  [F] T, if T PSSECT writes list to *_assemblages.txt
replicate_label  0.250  0->1 [0.025]
field_label_scale  0.75  [0.72] (rel)
font            Helvetica
grid           F  [F] T
half_ticks     T  [T] F
line_width     1.00  0-99 [1.] (pts)
picture_transformation :
      0.180 [0.18] x-scale (rel)
      0.180 [0.18] y-scale (rel)
      130.  [0.18] x-translation (pts)
      220.  [0.18] y-translation (pts)
      0.00  [0.0] rotation (deg)
plot_aspect_ratio  1.000  [1.0] x_axis_length/y_axis_length
splines         T  [T] F
tenth_ticks     F  [F] T
text_scale     1.000  [1.] (rel)
plot_extra_data
```

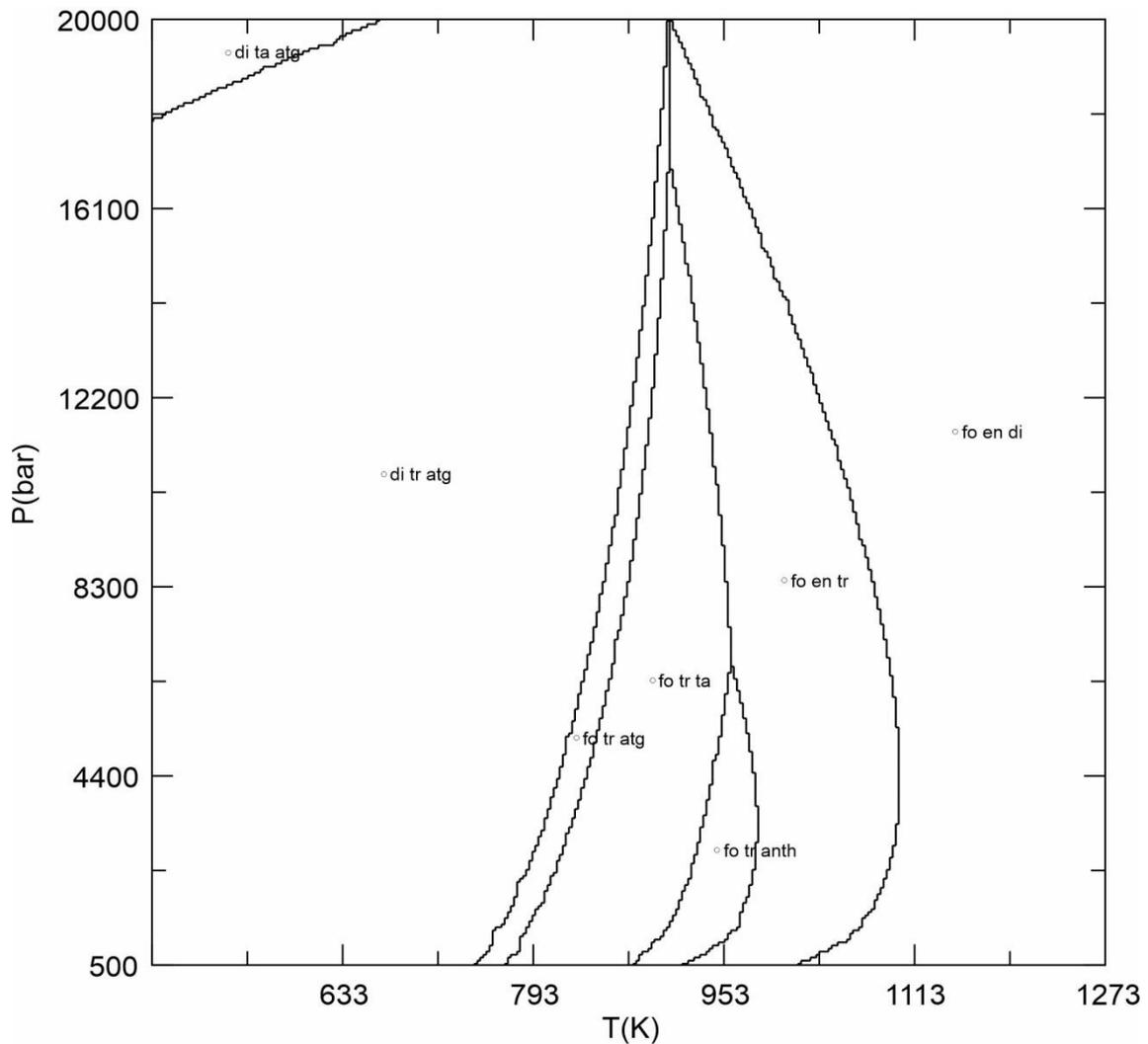
To change these options edit or create the plot option file

See: www.perplex.ethz.ch/perplex_plot_options.html

PostScript will be written to file: ex4.ps

Modify the default plot (y/n)?

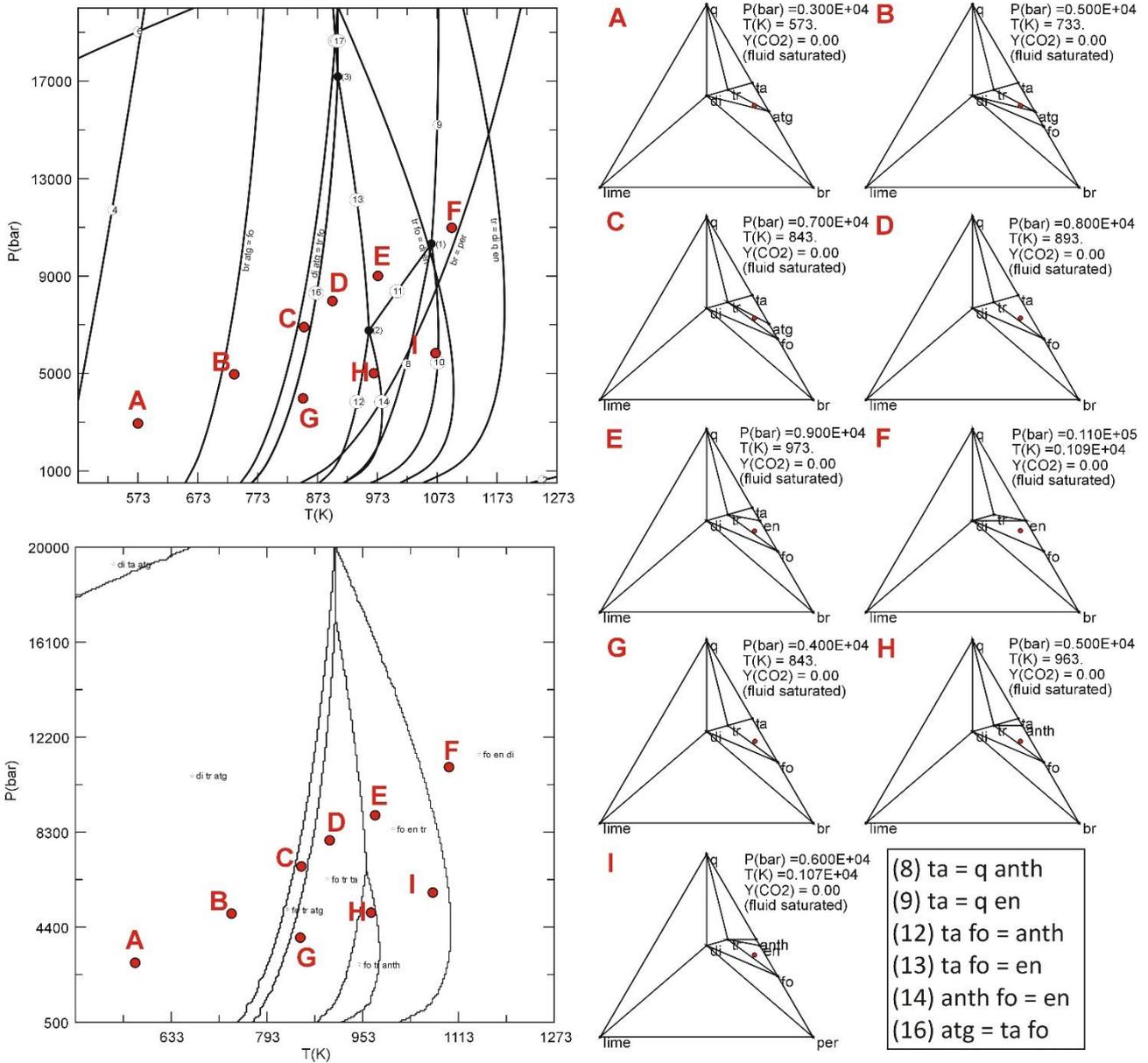
```
n
```



Being a very simple pseudosection (no solid solutions!), the stability fields of each mineral assemblage are separated by “real” reaction curves, i.e. UNIVARIANT CURVES, and all the field assemblages have the same variance. However, this is a very special case: pseudosections generally contain multi-variant field assemblages.

NB. The variance of each field is 2 [$f = c - p + 2$; $c = 4$ (CMSH); $p = 4$ (remember that each field also contains H_2O)]

(4) Comparison between projection and pseudosection



Comparison between the CSMH projection (Ex. 2) and the pseudosection (Ex. 4) calculated for a bulk composition $\text{MgO}=50 \text{ mol\%}$, $\text{SiO}_2=45 \text{ mol\%}$, $\text{CaO}=5 \text{ mol\%}$ (red dot in the chemographies – Ex. 3).

This specific bulk composition “sees” (i.e. is sensible to) only some of the reactions predicted by the P-T projection.

Ex 5

Ex. 5 – T-X(CO₂) projections and pseudosections for the CMS-H₂O-CO₂ system (no solid solutions)

This exercise investigates prograde metamorphism of impure dolomites and limestones characterized by different amounts of Cal, Dol and Qtz. A constant pressure of 1 kbar, typical of shallow level contact aureoles, is considered.

This exercise is useful to understand the difference between T-X(CO₂) projections and T-X(CO₂) pseudosections and allows you to become familiar with the use of H₂O-CO₂ fluids.

Ex. 5.1 – Isobaric T-X(CO₂) projection for a generic siliceous dolomite containing excess Cal

(1) Definition of the problem (BUILD)

```
C:\PERPLEX\Perplex691>build
```

Perple_X version 6.9.1, source updated January 3, 2022.

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NO is the default (blank) answer to all Y/N prompts

Enter a name for this project (the name will be used as the root for all output file names) [default = my_project]:

```
ex5_1
```

The problem definition file will be named: ex5_1.dat

Enter thermodynamic data file name [default = hp02ver.dat]:

```
hp62ver.dat
```

Enter the computational option file name [default = perplex_option.dat]:

See: www.perplex.ethz.ch/perplex_options.html

```
enter
```

Reading Perple_X options from: perplex_option.dat

The current data base components are:

Na2O MgO Al2O3 SiO2 K2O CaO TiO2 MnO FeO NiO ZrO2 Cl2 O2 H2O CO2 CuO Cr2O3 S2 F2 N2 ZnO

Transform them (Y/N)?

```
n
```

Specify computational mode:

- 1 - Convex-Hull minimization
- 2 - Constrained minimization on a 2d grid [default]
- 3 - Constrained minimization on a 1d grid
- 4 - Output pseudocompound data

5 - 1-d Phase fractionation

6 - 0-d Infiltration-reaction-fractionation

7 - 2-d Phase fractionation (FRAC2D and TITRATE reactive transport models)

Use Convex-Hull minimization for Schreinemakers projections or phase diagrams with > 2 independent variables. Use constrained minimization for phase diagrams or phase diagram sections with < 3 independent variables.

1

Calculations with a saturated fluid (Y/N)?

Y

Select the independent saturated fluid components:

H2O CO2

Enter names, 1 per line, press <enter> to finish:

For C-O-H fluids it is only necessary to select volatile species present in the solids of interest. If the species listed here are H2O and CO2, then to constrain O2 chemical potential to be consistent with C-O-H fluid speciation treat O2 as a saturated component. Refer to the Perple_X Tutorial for details.

H2O

CO2

Because we want to calculate a T-XCO2 grid, both H2O and CO2 must be included in the calculation.

Calculations with saturated components (Y/N)?

Y

We want to calculate the T-XCO2 grid with **calcite in excess**, therefore we must consider CaO as a saturated component.

****warning ver015**** if you select > 1 saturated component, then the order you enter the components determines the saturation heirarchy and may effect your results (see Connolly 1990).

NOTE: If more than one saturated component is specified Perple_X applies the constraints sequentially.

For example, if CaO and MgO are specified as saturated components in this order, this implies that calcite and dolomite would be excess phases; if the order is reversed (MgO, CaO) then, at the same conditions, the stable phases would be magnesite and calcite. This sequence is referred to as the saturation hierarchy.

Select < 6 saturated components from the set:

Na2O MgO Al2O3 SiO2 K2O CaO TiO2 MnO FeO NiO ZrO2 Cl2 O2 CuO Cr2O3 S2 F2 N2 ZnO

Enter names, 1 per line, press <enter> to finish:

CaO

Use chemical potentials, activities or fugacities as independent variables (Y/N)?

n

Select thermodynamic components from the set:

Na2O Al2O3 SiO2 K2O TiO2 MnO FeO NiO ZrO2 Cl2 O2 CuO Cr2O3 S2 F2 N2 ZnO

Enter names, 1 per line, press <enter> to finish:

MgO

SiO2

Because the thermodynamic data file identifies: H2O CO2 as special components, you will be prompted next for the EoS to be used for the corresponding composants and mixtures thereof. To override this behavior, e.g., to use a generic hybrid fluid EoS, delete the special_component section from the thermodynamic data file header.

NOTE: the EoS choice specified here will override the EoS choice specified by the hybrid_EoS option, to override this behavior delete the special_component section from the the thermodynamic data file header.

Select fluid equation of state:

- 0 - X(CO2) H2O-CO2 Modified Redlich-Kwong (MRK) DeSantis et al 74
- 1 - X(CO2) H2O-CO2 HSMRK Kerrick & Jacobs 81
- 2 - X(CO2) H2O-CO2 MRK hybrid-EoS*
- 5 - X(CO2) H2O-CO2 CORK Holland & Powell 91, 98
- 8 - f(O2/CO2) C-buffered COH MRK hybrid-EoS*
- 10 - X(O) C-buffered COH MRK hybrid-EoS Connolly & Cesare 93*
- 12 - X(O)-f(S2) C-buffered COHS MRK hybrid-EoS Connolly & Cesare 93*
- 13 - X(H2) H2O-H2 MRK hybrid-EoS*
- 14 - X(CO2) H2O-CO2 Pitzer & Sterner 94; Holland & Powell mixing 03
- 15 - X(H2) H2O-H2 low T MRK hybrid-EoS*
- 16 - X(O) H-O MRK hybrid-EoS*
- 17 - X(O)-f(S2) H-O-S MRK hybrid-EoS*
- 19 - X(O)-X(S) C-buffered COHS MRK hybrid-EoS Connolly & Cesare 93*
- 20 - X(O)-X(C) COHS MRK hybrid-EoS Connolly & Cesare 93*
- 24 - f(O2/CO2)-N/C C-buffered COHN MRK hybrid-EoS*
- 25 - X(CO2)-X(NaCl) H2O-CO2-NaCl Aranovich et al 10
- 26 - X(O) O-Si MRK Connolly 16
- 27 - X(O)-X(C) C-O-H MRK hybrid-EoS*

*Hybrid EoS use the following pure species EoS, to change these associations modify the hybrid_EoS keywords in the perplex_option file:

- H2O - PSEoS Pitzer & Sterner 1994
- CO2 - PSEoS Pitzer & Sterner 1994
- CH4 - MRK DeSantis et al 1974

5

The data base has P(bar) and T(K) as default independent potentials.

Make one dependent on the other, e.g., as along a geothermal gradient (y/n)?

n

Specify number of independent potential variables:

- 0 - Composition diagram [default]
- 1 - Mixed-variable diagram
- 2 - Sections and Schreinemakers-type diagrams

2

Select x-axis variable:

- 1 - P(bar)
- 2 - T(K)
- 3 - Y(CO2)

3

Enter minimum and maximum values, respectively, for: Y(CO2)

0.00001

1

CONVEX might not be able to trace equilibria which occur at very low XCO2 values ($XCO_2 < 1 \text{ e-}6$); therefore, it is suggested to set a XCO2 minim value different from 0 (e.g. 0.00001)

Select y-axis variable:

2 - T(K)

3 - P(bar)

2

Enter minimum and maximum values, respectively, for: T(K)

573

873

Specify sectioning value for: P(bar)

1000

Output a print file (Y/N)?

y

Exclude pure and/or endmember phases (Y/N)?

y

Do you want to be prompted for phases (Y/N)?

n

Enter names, 1 per line, press <enter> to finish:

At very low XCO₂ values, equilibria involving Ca- and/or Mg-rich silicates such as rankinite, larnite, akermanite, merwinite, spurrite tyllite, monticellite, chlinohumite, clinohumite and clinoenstatite could become metastable, therefore their exclusion is meaningful.

rnk	rankinite Ca ₃ Si ₂ O ₇
lrn	larnite Ca ₂ SiO ₄
cstn	"Si-titanite" CaSi ₂ O ₅ (one Si replaces Ti)
ty	tilleyte Ca ₅ Si ₂ O ₇ (CO ₃) ₂
spu	spurrite Ca ₅ Si ₂ O ₈ (CO ₃)
ak	akermanite Ca ₂ MgSi ₂ O ₇
merw	merwinite Ca ₃ MgSi ₂ O ₈
mont	monticellite CaMgSiO ₄
chum	clinohumite Mg ₉ Si ₄ O ₁₆ (OH) ₂
cen	clinoenstatite Mg ₂ Si ₂ O ₆

Include solution models (Y/N)?

n

Enter calculation title:

ex5_1

(2) Doing the calculation (CONVEX)

Run CONVEX to make the calculation:

C:\PERPLEX\Perplex691>convex

Perple_X version 6.9.1, source updated January 3, 2022.

Enter the project name (the name assigned in BUILD) [default = my_project]:

ex5_1

Reading problem definition from file: ex5_1.dat
Reading thermodynamic data from file: hp62ver.dat
Writing print output to file: ex5_1.plt
Writing plot output to file: ex5_1.plt
Reading solution models from file: not requested
Reading Perple_X options from: perplex_option.dat
Writing complete reaction list to: not requested
Writing Perple_X option summary to: not requested

Perple_X computational option settings for CONVEX:

Keyword: Value: Permitted values [default]:

Auto-refine options:

auto_refine aut [auto] manual off
replicate_threshold 0.1E-1 [1e-2]; static opt; <0 => no replica test
rep_dynamic_threshold 0.1E-2 [1d-3]; dynamic opt; <0 => no replica test
re-refine F [F] T
intermediate_savrpc F [F] T
intermediate_savdyn F [F] T
keep_all_rpcs T [T] F

Schreinemakers and Mixed-variable diagram options:

variance 1/99 [1/99], >0; maximum true variance
increment 0.100/0.025 [0.1/0.025], default search/trace variable increment
efficiency 3 [3] >0, <6
reaction_format min [min] full stoichiometry S+V everything
reaction_list off [off] on
console_messages on [on] off
short_print_file on [on] off

Solution subdivision options:

initial_resolution:
exploratory stage 0.0625 0->1 [1/16], 0 => off
auto-refine stage 0.0208 0->1 [], 0 => off
stretch_factor 0.0020 >0 [2d-3]
non_linear_switch F [F] T
subdivision_override off [off] lin str
hard_limits off [off] on
refine_endmembers F [F] T
pc_perturbation 0.0050 [5d-3]

Thermodynamic options:

solvus_tolerance aut [aut] or 0->1; aut = automatic, 0 => p=c pseudocompounds, 1 => homogenize
T_stop (K) 0.0 [0]
T_melt (K) 873.0 [873]
approx_alpha T [T] F
Anderson-Gruneisen F [F] T
speciation_precision 0.1E-4 [1d-5] <1; absolute
speciation_max_it 100 [100]
GFSM F [F] T GFSM/special_component toggle

```

hybrid_EoS_H2O      4      [4] 0-2, 4-7
hybrid_EoS_CO2      4      [4] 0-4, 7
hybrid_EoS_CH4      0      [0] 0-1, 7
aq_bad_results      err    [err] 101 102 103 ignore
aq_lagged_speciation F      [F] T
aq_ion_H+           T      [T] F => use OH-
aq_oxide_components F      [F] T
aq_solvent_solvus   T      [T] F
aq_vapor_epsilon    1.0    [1.]

```

Input/Output options:

```

pause_on_error      T      [T] F
timing               T      [T] F
auto_exclude        T      [T] F

```

To change these options see: www.perplex.ethz.ch/perplex_options.html

Summary of make-definition entities:

```

cumm_dqf fo8L q8L cenjh odi qjL dijL fojL foTL mcpv cmpv foHL qHL

```

Summary of saturated-component entities:

for: CaO

```

lime cc arag limL

```

**** Starting auto_refine computational stage ****

```

cycle      1      1      1
cycle      2      2      2
cycle      3      3      3

```

Initial number of divariant assemblages to be tested is: 3

Testing divariant assemblage 1, 2 assemblages remaining to be tested.

****warning ver079**** univeq failed on an edge for the following equilibrium.

Probable cause is extreme independent variable limits (e.g., xco2=0) or poor convergence criteria in the thermodynamic data file. In routine:COFACE

finished with equilibrium (1) dol = br

Testing divariant assemblage 2, 2 assemblages remaining to be tested.

****warning ver079**** univeq failed on an edge for the following equilibrium.

Probable cause is extreme independent variable limits (e.g., xco2=0) or poor convergence criteria in the thermodynamic data file. In routine:COFACE

finished with equilibrium (2) tr = atg di

Testing divariant assemblage 3, 3 assemblages remaining to be tested.

finished with equilibrium (3) q = wo

finished with equilibrium (4) di = wo fo

finished with equilibrium (5) di = wo br

****warning ver047**** univariant field 6 terminates at an invariant field that could not be located within the tolerance specified in the thermodynamic data file (PTOL= 0.300000E-02).

finished with equilibrium (6) di br = fo

finished with equilibrium (6) di br = fo

finished with equilibrium (7) fo = wo br

****warning ver047**** univariant field 8 terminates at an invariant field that could not be located within the tolerance specified in the thermodynamic data file (PTOL= 0.300000E-02).

finished with equilibrium (8) atg = di fo

finished with equilibrium (8) atg = di fo
finished with equilibrium (9) atg = di br
warning ver047 univariant field 10 terminates at an invariant field that could not be located within the tolerance specified in the thermodynamic data file (PTOL= 0.300000E-02).
finished with equilibrium (10) br atg = fo
warning ver047 univariant field 10 terminates at an invariant field that could not be located within the tolerance specified in the thermodynamic data file (PTOL= 0.300000E-02).
finished with equilibrium (10) br atg = fo
warning ver047 univariant field 10 terminates at an invariant field that could not be located within the tolerance specified in the thermodynamic data file (PTOL= 0.300000E-02).
finished with equilibrium (10) br atg = fo
finished with equilibrium (10) br atg = fo
finished with equilibrium (11) tr = di fo
finished with equilibrium (2) tr = di atg
warning ver047 univariant field 12 terminates at an invariant field that could not be located within the tolerance specified in the thermodynamic data file (PTOL= 0.300000E-02).
finished with equilibrium (12) atg = fo tr
finished with equilibrium (12) atg = fo tr
finished with equilibrium (1) dol = br
finished with equilibrium (13) atg dol = fo
finished with equilibrium (1) dol = br
finished with equilibrium (14) di dol = fo
finished with equilibrium (15) tr = di dol
finished with equilibrium (16) tr dol = fo
finished with equilibrium (17) tr dol = atg
warning ver020 sfol2
finished with equilibrium (18) tr q = di
finished with equilibrium (19) dol q = di
finished with equilibrium (20) dol q = tr
finished with equilibrium (21) ta = atg tr
finished with equilibrium (22) dol ta = atg
finished with equilibrium (23) ta = tr dol
finished with equilibrium (24) q ta = tr
finished with equilibrium (25) dol q = ta
warning ver074 no new equilibria identified, if degenerate segments have been skipped increase the computational reliability level.
Testing divariant assemblage 4, 4 assemblages remaining to be tested.
Testing divariant assemblage 5, 4 assemblages remaining to be tested.
finished with equilibrium (18) tr q = di
Testing divariant assemblage 6, 4 assemblages remaining to be tested.
Testing divariant assemblage 7, 5 assemblages remaining to be tested.
Testing divariant assemblage 8, 4 assemblages remaining to be tested.
Testing divariant assemblage 9, 4 assemblages remaining to be tested.
Testing divariant assemblage 10, 4 assemblages remaining to be tested.
Testing divariant assemblage 11, 4 assemblages remaining to be tested.
warning ver066 Metastable assemblage into FLIPIT:
ta atg
v = 1000.00 573.000 0.782242E-02 0.00000 0.00000
Testing divariant assemblage 12, 3 assemblages remaining to be tested.
Testing divariant assemblage 13, 2 assemblages remaining to be tested.
Testing divariant assemblage 14, 3 assemblages remaining to be tested.

Testing divariant assemblage	15,	4 assemblages remaining to be tested.
Testing divariant assemblage	16,	4 assemblages remaining to be tested.
Testing divariant assemblage	17,	5 assemblages remaining to be tested.
Testing divariant assemblage	18,	4 assemblages remaining to be tested.
Testing divariant assemblage	19,	3 assemblages remaining to be tested.
Testing divariant assemblage	20,	4 assemblages remaining to be tested.
Testing divariant assemblage	21,	4 assemblages remaining to be tested.
Testing divariant assemblage	22,	3 assemblages remaining to be tested.
Testing divariant assemblage	23,	2 assemblages remaining to be tested.
Testing divariant assemblage	24,	2 assemblages remaining to be tested.
Testing divariant assemblage	25,	1 assemblages remaining to be tested.
Testing divariant assemblage	26,	0 assemblages remaining to be tested.

 WARNING!! The stability fields of the following equilibria may have been entirely or partially skipped in the calculation:

(1-1) dol = br
 (2-1) tr = di atg

(3) Plotting the calculated phase diagram (PSVDRAW)

Run PSVDRAW to plot the calculated phase diagram:

C:\PERPLEX\Perplex691>psvdraw

Perple_X version 6.9.1, source updated January 3, 2022.

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Enter the project or plot file name [i.e., without the .plt suffix]:

ex5_1

Perple_X plot options are currently set as:

Keyword:	Value:	Permitted values [default]:
axis_label_scale	1.20	[1.2] (rel)
bounding_box :		
	0	[0] x-min (pts)
	0	[0] y-min (pts)
	800	[800] x-length (pts)
	800	[800] y-length (pts)
field_fill	T	[T] F
field_label	T	[T] F
numeric_field_label	F	[F] T, if T PSSECT writes list to *_assemblages.txt
replicate_label	0.250	0->1 [0.025]
field_label_scale	0.75	[0.72] (rel)
font	Helvetica	
grid	F	[F] T
half_ticks	T	[T] F
line_width	1.00	0-99 [1.] (pts)
picture_transformation :		
	0.180	[0.18] x-scale (rel)
	0.180	[0.18] y-scale (rel)

```

130. [0.18] x-translation (pts)
220. [0.18] y-translation (pts)
0.00 [0.0] rotation (deg)
plot_aspect_ratio 1.000 [1.0] x_axis_length/y_axis_length
splines T [T] F
tenth_ticks F [F] T
text_scale 1.000 [1.] (rel)
plot_extra_data

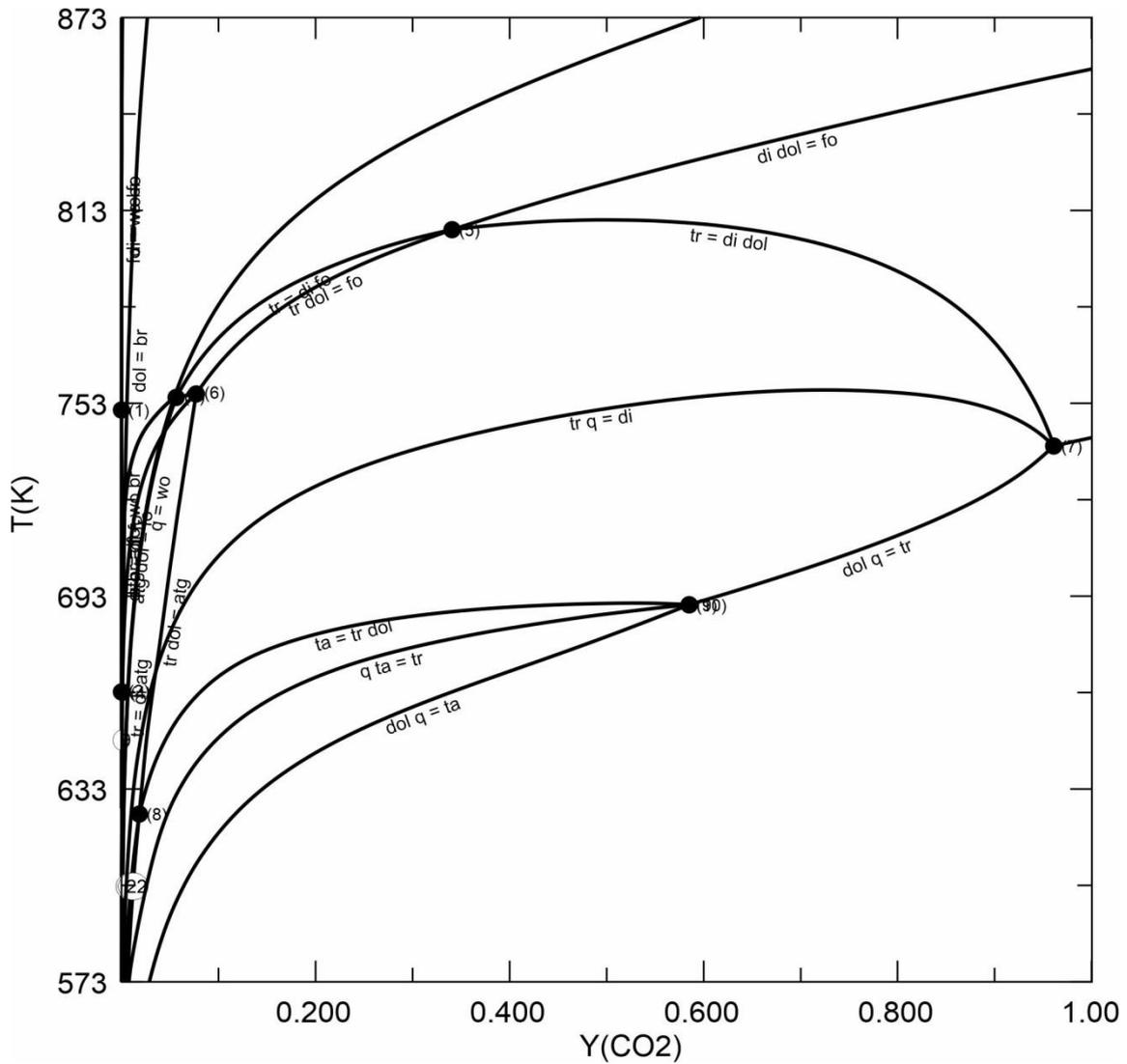
```

To change these options edit or create the plot option file
 See: www.perplex.ethz.ch/perplex_plot_options.html

PostScript will be written to file: ex5_1.ps

Modify the default plot (y/n)?

N



Ex. 5.2 – Isobaric T-XCO₂ pseudosection of a siliceous dolomite for the composition 2Qtz–2Dol–1Cal (see Bucher & Grapes, 2011; Fig. 6.8)

(1) Definition of the problem (BUILD)

C:\PERPLEX\Perplex691>build

Perple_X version 6.9.1, source updated January 3, 2022.

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NO is the default (blank) answer to all Y/N prompts

Enter a name for this project (the name will be used as the root for all output file names) [default = my_project]:

ex5_2

The problem definition file will be named: ex5_2.dat

Enter thermodynamic data file name [default = hp02ver.dat]:

hp62ver.dat

Enter the computational option file name [default = perplex_option.dat]:

See: www.perplex.ethz.ch/perplex_options.html

Reading Perple_X options from: perplex_option.dat

The current data base components are:

Na2O MgO Al2O3 SiO2 K2O CaO TiO2 MnO FeO NiO ZrO2 I2 O2 H2O CO2 CuO Cr2O3 S2 F2 N2 ZnO

Transform them (Y/N)?

n

Specify computational mode:

- 1 - Convex-Hull minimization
- 2 - Constrained minimization on a 2d grid [default]
- 3 - Constrained minimization on a 1d grid
- 4 - Output pseudocompound data
- 5 - 1-d Phase fractionation
- 6 - 0-d Infiltration-reaction-fractionation
- 7 - 2-d Phase fractionation (FRAC2D and TITRATE reactive transport models)

Use Convex-Hull minimization for Schreinemakers projections or phase diagrams with > 2 independent variables. Use constrained minimization for phase diagrams or phase diagram sections with < 3 independent variables.

2

Calculations with a saturated fluid (Y/N)?

y

Select the independent saturated fluid components:

H2O CO2

Enter names, 1 per line, press <enter> to finish:

For C-O-H fluids it is only necessary to select volatile species present in the solids of interest. If the species listed here are H2O and CO2, then to constrain O2 chemical potential to be consistent with C-O-H fluid speciation treat O2 as a saturated component. Refer to the Perple_X Tutorial for details.

H2O

CO2

Calculations with saturated components (Y/N)?

n

Use chemical potentials, activities or fugacities as independent variables (Y/N)?

n

Select thermodynamic components from the set:

Na2O MgO Al2O3 SiO2 K2O CaO TiO2 MnO FeO NiO ZrO2 Cl2 O2 CuO Cr2O3 S2 F2

Enter names, 1 per line, press <enter> to finish:

MgO

CaO

SiO2

Because the thermodynamic data file identifies: H2O CO2 as special components, you will be prompted next for the EoS to be used for the corresponding components and mixtures thereof. To override this behavior, e.g., to use a generic hybrid fluid EoS, delete the special_component section from the thermodynamic data file header.

NOTE: the EoS choice specified here will override the EoS choice specified by the hybrid_EoS option, to override this behavior delete the special_component section from the the thermodynamic data file header.

Select fluid equation of state:

0 - X(CO2) H2O-CO2 Modified Redlich-Kwong (MRK) DeSantis et al 74

1 - X(CO2) H2O-CO2 HSMRK Kerrick & Jacobs 81

2 - X(CO2) H2O-CO2 MRK hybrid-EoS*

5 - X(CO2) H2O-CO2 CORK Holland & Powell 91, 98

8 - f(O2/CO2) C-buffered COH MRK hybrid-EoS*

10 - X(O) C-buffered COH MRK hybrid-EoS Connolly & Cesare 93*

12 - X(O)-f(S2) C-buffered COHS MRK hybrid-EoS Connolly & Cesare 93*

13 - X(H2) H2O-H2 MRK hybrid-EoS*

14 - X(CO2) H2O-CO2 Pitzer & Sterner 94; Holland & Powell mixing 03

15 - X(H2) H2O-H2 low T MRK hybrid-EoS*

16 - X(O) H-O MRK hybrid-EoS*

17 - X(O)-f(S2) H-O-S MRK hybrid-EoS*

19 - X(O)-X(S) C-buffered COHS MRK hybrid-EoS Connolly & Cesare 93*

20 - X(O)-X(C) COHS MRK hybrid-EoS Connolly & Cesare 93*

24 - f(O2/CO2)-N/C C-buffered COHN MRK hybrid-EoS*

25 - X(CO2)-X(NaCl) H2O-CO2-NaCl Aranovich et al 10

26 - X(O) O-Si MRK Connolly 16

27 - X(O)-X(C) C-O-H MRK hybrid-EoS*

*Hybrid EoS use the following pure species EoS, to change these associations modify the hybrid_EoS keywords in the perplex_option file:

H2O - PSEoS Pitzer & Sterner 1994

CO2 - PSEoS Pitzer & Sterner 1994

5

The data base has P(bar) and T(K) as default independent potentials.
Make one dependent on the other, e.g., as along a geothermal gradient (y/n)?

n

Select x-axis variable:

- 1 - P(bar)
- 2 - T(K)
- 3 - Y(CO2)
- 4 - Composition X_C1* (user defined)

*X_C1 can not be selected as the y-axis variable

3

Enter minimum and maximum values, respectively, for: Y(CO2)

0.00001

1

Select y-axis variable:

- 2 - T(K)
- 3 - P(bar)

2

Enter minimum and maximum values, respectively, for: T(K)

573

873

Specify sectioning value for: P(bar)

1000

For gridded minimization, grid resolution is determined by the number of levels (grid_levels) and the resolution at the lowest level in the X- and Y-directions (x_nodes and y_nodes) these parameters are currently set for the exploratory and autorefine cycles as follows:

stage	grid_levels	xnodes	ynodes	effective resolution
exploratory	1	10	10	10 x 10 nodes
auto-refine	4	40	40	313 x 313 nodes

To change these options edit or create the file perplex_option.dat

See: www.perplex.ethz.ch/perplex_options.html#grid_parameters

Specify component amounts by mass (Y/N)?

n

The amounts you enter next need not be normalized; regardless of units, they define the molar amount of the system

The starting composition 2Qtz + 2Dol + 1Cal means: 2SiO₂ + 2MgO + 3CaO

Enter the molar amounts of the components:

MgO CaO SiO₂

for the bulk composition of interest:

2
3
2

Output a print file (Y/N)?

Y

Exclude pure and/or endmember phases (Y/N)?

Y

Do you want to be prompted for phases (Y/N)?

N

Enter names, 1 per line, press <enter> to finish:

Same as in Ex. 5_1:

rnk	rankinite Ca ₃ Si ₂ O ₇
lrn	larnite Ca ₂ SiO ₄
cstn	"Si-titanite" CaSi ₂ O ₅ (one Si replaces Ti)
ty	tilleyte Ca ₅ Si ₂ O ₇ (CO ₃) ₂
spu	spurrite Ca ₅ Si ₂ O ₈ (CO ₃)
ak	akermanite Ca ₂ MgSi ₂ O ₇
merw	merwinite Ca ₃ MgSi ₂ O ₈
mont	monticellite CaMgSiO ₄
chum	clinohumite Mg ₉ Si ₄ O ₁₆ (OH) ₂
cen	clinoenstatite Mg ₂ Si ₂ O ₆

Include solution models (Y/N)?

n

Enter calculation title:

ex5_2

(2) Doing the calculation (VERTEX)

Run VERTEX to make the calculation:

```
C:\PERPLEX\Perplex691>vertex
```

Perple_X version 6.9.1, source updated January 3, 2022.

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Enter the project name (the name assigned in BUILD) [default = my_project]:

ex5_2

Reading problem definition from file: ex5_2.dat

Reading thermodynamic data from file: hp62ver.dat

Writing print output to file: ex5_2.plt

Writing plot output to file: ex5_2.plt

Writing phase assemblage data to file: ex5_2.blk
Reading solution models from file: not requested
Reading Perple_X options from: perplex_option.dat
Writing seismic data options to: ex5_2_seismic_data.txt
Writing Perple_X option summary to: not requested

Perple_X computational option settings for VERTEX:

Keyword: Value: Permitted values [default]:

Auto-refine options:

auto_refine aut [auto] manual off
replicate_threshold 0.1E-1 [1e-2]; static opt; <0 => no replica test
rep_dynamic_threshold 0.1E-2 [1d-3]; dynamic opt; <0 => no replica test
re-refine F [F] T
intermediate_savrpc F [F] T
intermediate_savdyn F [F] T
keep_all_rpc T [T] F

Free energy minimization options:

MINFRC_diff_increment 0.1E-6 [1e-7] 1e-3 => 1e-9
MINFXC_solver 0 [0] >= 0 - speci2, -1 - MINFXC
optimization_max_it 40 [40] >1
optimization_precision 0.1E-3 [1e-4], 1e-1 => 1e-6, absolute
order_check F [F] T
refinement_points 5 [auto] 1->14
refinement_switch F [T] F
scatter-points T [T] F
scatter-increment 0.1E-1 [1e-2] 1e-2 => 1e-7
solvus_tolerance_ll aut [0.2] 0->1
zero_mode 0.1E-5 [1e-6] 0->1; < 0 => off

2D grid options:

x_nodes 10 / 40 [10/40] >0, <2048; effective x-resolution 10 / 313 nodes
y_nodes 10 / 40 [10/40] >0, <2048; effective y-resolution 10 / 313 nodes
grid_levels 1 / 4 [1/4] >0, <10
linear_model on [on] off

Solution subdivision options:

initial_resolution: 0.2500 [1/4] 0->1; 0 => off
stretch_factor 0.0020 [2d-3] >0
non_linear_switch F [F] T
subdivision_override off [lin] off str
refine_endmembers F [F] T

Thermodynamic options:

solvus_tolerance aut [aut] or 0->1; aut = automatic, 0 => p=c pseudocompounds, 1 => homogenize
T_stop (K) 0.0 [0]
T_melt (K) 873.0 [873]
approx_alpha T [T] F
Anderson-Gruneisen F [F] T
speciation_precision 0.1E-4 [1d-5] <1; absolute
speciation_max_it 100 [100]
GFSM F [F] T GFSM/special_component toggle
hybrid_EoS_H2O 4 [4] 0-2, 4-7
hybrid_EoS_CO2 4 [4] 0-4, 7
hybrid_EoS_CH4 0 [0] 0-1, 7

aq_bad_results err [err] 101 102 103 ignore
aq_lagged_speciation F [F] T
aq_ion_H+ T [T] F => use OH-
aq_oxide_components F [F] T
aq_solvent_solvus T [T] F
aq_vapor_epsilon 1.0 [1.]

Input/Output options:

pause_on_error T [T] F
timing T [T] F
auto_exclude T [T] F
logarithmic_p F [F] T
bad_number NaN [NaN]
interim_results aut [auto] off manual

Information file output options:

option_list_files F [F] T; echo computational options
pseudocompound_file F [F] T; echo static pseudocompound compositions
auto_refine_file F [T] F; echo auto-refine compositions
seismic_data_file T [F] T; echo seismic wavespeed options

To change these options see: www.perplex.ethz.ch/perplex_options.html

Summary of make-definition entities:

cumm_dqf fo8L q8L cenjh odi qjL dijL fojL foTL mcpv cmpv foHL qHL

warning ver099 no data for aqueous species, aq_output and aq_lagged_speciation disabled.

** Starting exploratory computational stage **

2.5% done with low level grid.
5.0% done with low level grid.
7.5% done with low level grid.
10.0% done with low level grid.
12.5% done with low level grid.
15.0% done with low level grid.
17.5% done with low level grid.
20.0% done with low level grid.
22.5% done with low level grid.
25.0% done with low level grid.
27.5% done with low level grid.
30.0% done with low level grid.
32.5% done with low level grid.
35.0% done with low level grid.
37.5% done with low level grid.
40.0% done with low level grid.
42.5% done with low level grid.
45.0% done with low level grid.
47.5% done with low level grid.
50.0% done with low level grid.
52.5% done with low level grid.
55.0% done with low level grid.
57.5% done with low level grid.
60.0% done with low level grid.
62.5% done with low level grid.
65.0% done with low level grid.

67.5% done with low level grid.
70.0% done with low level grid.
72.5% done with low level grid.
75.0% done with low level grid.
77.5% done with low level grid.
80.0% done with low level grid.
82.5% done with low level grid.
85.0% done with low level grid.
87.5% done with low level grid.
90.0% done with low level grid.
92.5% done with low level grid.
95.0% done with low level grid.
97.5% done with low level grid.
100.0% done with low level grid.

Beginning grid refinement stage.

234 grid cells to be refined at grid level 2

...working (502 minimizations done)

refinement at level 2 involved 534 minimizations

2134 minimizations required of the theoretical limit of 6241

461 grid cells to be refined at grid level 3

...working (470 minimizations done)

...working (971 minimizations done)

refinement at level 3 involved 975 minimizations

3109 minimizations required of the theoretical limit of 24649

916 grid cells to be refined at grid level 4

...working (498 minimizations done)

...working (1000 minimizations done)

...working (1501 minimizations done)

refinement at level 4 involved 1893 minimizations

5002 minimizations required of the theoretical limit of 98596

Exploratory stage generated:

Total number of compositions: 0

** Starting auto-refine computational stage **

2.5% done with low level grid.
5.0% done with low level grid.
7.5% done with low level grid.
10.0% done with low level grid.
12.5% done with low level grid.
15.0% done with low level grid.
17.5% done with low level grid.
20.0% done with low level grid.
22.5% done with low level grid.
25.0% done with low level grid.
27.5% done with low level grid.
30.0% done with low level grid.
32.5% done with low level grid.
35.0% done with low level grid.
37.5% done with low level grid.

40.0% done with low level grid.
 42.5% done with low level grid.
 45.0% done with low level grid.
 47.5% done with low level grid.
 50.0% done with low level grid.
 52.5% done with low level grid.
 55.0% done with low level grid.
 57.5% done with low level grid.
 60.0% done with low level grid.
 62.5% done with low level grid.
 65.0% done with low level grid.
 67.5% done with low level grid.
 70.0% done with low level grid.
 72.5% done with low level grid.
 75.0% done with low level grid.
 77.5% done with low level grid.
 80.0% done with low level grid.
 82.5% done with low level grid.
 85.0% done with low level grid.
 87.5% done with low level grid.
 90.0% done with low level grid.
 92.5% done with low level grid.
 95.0% done with low level grid.
 97.5% done with low level grid.
 100.0% done with low level grid.

Beginning grid refinement stage.

234 grid cells to be refined at grid level 2
 ...working (502 minimizations done)
 refinement at level 2 involved 534 minimizations
 2134 minimizations required of the theoretical limit of 6241
 461 grid cells to be refined at grid level 3
 ...working (470 minimizations done)
 ...working (971 minimizations done)
 refinement at level 3 involved 975 minimizations
 3109 minimizations required of the theoretical limit of 24649
 916 grid cells to be refined at grid level 4
 ...working (498 minimizations done)
 ...working (1000 minimizations done)
 ...working (1501 minimizations done)
 refinement at level 4 involved 1893 minimizations
 5002 minimizations required of the theoretical limit of 98596

Timing	min.	% of total
Static G calculation	0.36458E-02	13.7
Dynamic G calculation	0.0000	0.0
Static LP	0.78125E-03	2.9
Dynamic LP	0.0000	0.0
Successive QP	0.0000	0.0
Total of above	0.44271E-02	16.7
Total elapsed time	0.26562E-01	100.0

End of job: ex5_2

(3) Plotting the calculated phase diagram (PSSECT)

Run PSSECT to plot the calculated pseudosection:

```
C:\PERPLEX\Perplex691>pssect
```

Perple_X version 6.9.1, source updated January 3, 2022.

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Enter the project name (the name assigned in BUILD) [default = my_project]:

```
ex5_2
```

Reading Perple_X options from: perplex_option.dat

Perple_X plot options are currently set as:

Keyword:	Value:	Permitted values [default]:
axis_label_scale	1.20	[1.2] (rel)
bounding_box :		
	0	[0] x-min (pts)
	0	[0] y-min (pts)
	800	[800] x-length (pts)
	800	[800] y-length (pts)
field_fill	T	[T] F
field_label	T	[T] F
numeric_field_label	F	[F] T, if T PSSECT writes list to *_assemblages.txt
replicate_label	0.250	0->1 [0.025]
field_label_scale	0.75	[0.72] (rel)
font	Helvetica	
grid	F	[F] T
half_ticks	T	[T] F
line_width	1.00	0-99 [1.] (pts)
picture_transformation :		
	0.180	[0.18] x-scale (rel)
	0.180	[0.18] y-scale (rel)
	130.	[0.18] x-translation (pts)
	220.	[0.18] y-translation (pts)
	0.00	[0.0] rotation (deg)
plot_aspect_ratio	1.000	[1.0] x_axis_length/y_axis_length
splines	T	[T] F
tenth_ticks	F	[F] T
text_scale	1.000	[1.] (rel)
plot_extra_data		

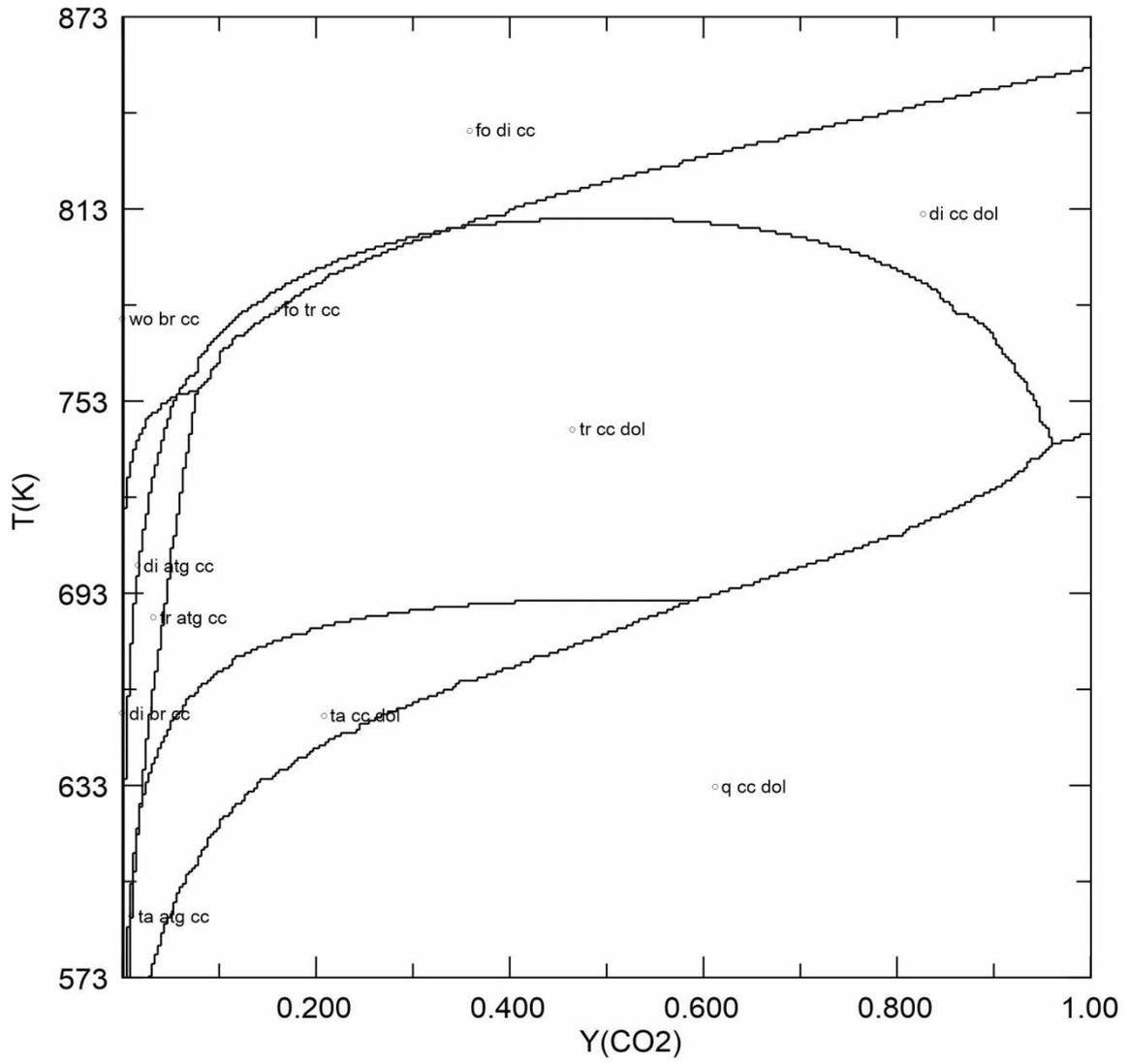
To change these options edit or create the plot option file

See: www.perplex.ethz.ch/perplex_plot_options.html

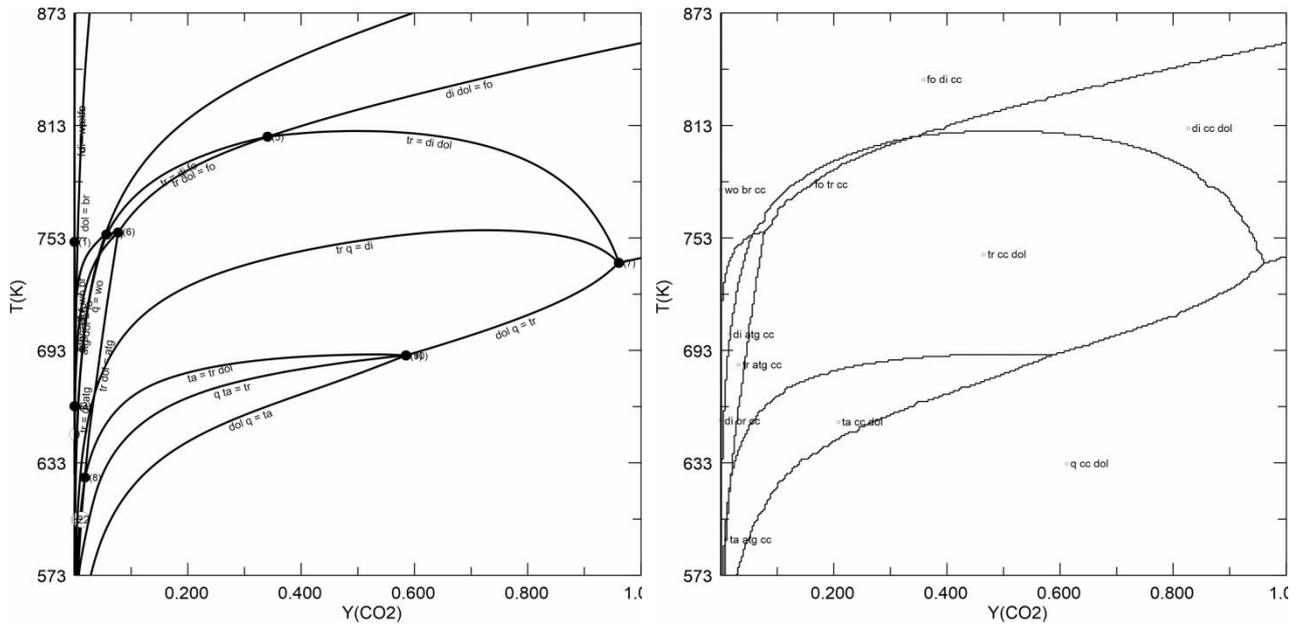
PostScript will be written to file: ex5_2.ps

Modify the default plot (y/n)?

N



Comparison between projections and pseudosections



Comparison between the isobaric $T-X(\text{CO}_2)$ projection for a generic siliceous dolomite containing excess calcite (Ex. 5.1) and the pseudosection calculated for a bulk composition $\text{MgO}=2$, $\text{CaO}=3$, $\text{SiO}_2=2$ mol% ($2\text{Qtz}+2\text{Dol}+1\text{Cal}$; Ex. 5.2). **This specific bulk composition “sees” (i.e. is sensible to) only some of the reactions predicted by the P-T projection.**

Ex. 5.3 – Isobaric T-X(CO₂) projection for a generic siliceous limestone containing excess Qtz

(1) Definition of the problem (BUILD)

The problem is the same as in Ex. 5.1, except for the choice of the excess component that is now SiO₂ (quartz is in excess). You can edit the `ex5_1.dat` input file (change the name in `ex5_3`). The thermodynamic components are now MgO and CaO, whereas the saturated component is SiO₂.

```
begin thermodynamic component list
MgO  0  0.00000      0.00000      0.00000      unconstrained amount
CaO  0  0.00000      0.00000      0.00000      unconstrained amount
end thermodynamic component list

begin saturated component list
SiO2  0  0.00000      0.00000      0.00000      unconstrained amount
end saturated component list
```

(2) Doing the calculation (CONVEX)

Run CONVEX to make the calculation:

```
C:\PERPLEX\Perplex691>convex
```

Perple_X version 6.9.1, source updated January 3, 2022.

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Enter the project name (the name assigned in BUILD) [default = my_project]:

```
ex5_3
```

```
Reading problem definition from file: ex5_3.dat
Reading thermodynamic data from file: hp62ver.dat
Writing print output to file: ex5_3.plt
Writing plot output to file: ex5_3.plt
Reading solution models from file: not requested
Reading Perple_X options from: perplex_option.dat
Writing complete reaction list to: not requested
Writing Perple_X option summary to: not requested
```

Perple_X computational option settings for CONVEX:

Keyword: Value: Permitted values [default]:

Auto-refine options:

```
auto_refine      aut  [auto] manual off
replicate_threshold  0.1E-1  [1e-2]; static opt; <0 => no replica test
rep_dynamic_threshold  0.1E-2  [1d-3]; dynamic opt; <0 => no replica test
re-refine        F    [F] T
intermediate_savrpc  F    [F] T
intermediate_savdyn  F    [F] T
keep_all_rpcs      T    [T] F
```

Schreinemakers and Mixed-variable diagram options:

variance 1/99 [1/99], >0; maximum true variance
increment 0.100/0.025 [0.1/0.025], default search/trace variable increment
efficiency 3 [3] >0, <6
reaction_format min [min] full stoichiometry S+V everything
reaction_list off [off] on
console_messages on [on] off
short_print_file on [on] off

Solution subdivision options:

initial_resolution:
exploratory stage 0.0625 0->1 [1/16], 0 => off
auto-refine stage 0.0208 0->1 [], 0 => off
stretch_factor 0.0020 >0 [2d-3]
non_linear_switch F [F] T
subdivision_override off [off] lin str
hard_limits off [off] on
refine_endmembers F [F] T
pc_perturbation 0.0050 [5d-3]

Thermodynamic options:

solvus_tolerance aut [aut] or 0->1; aut = automatic, 0 => p=c pseudocompounds, 1 => homogenize
T_stop (K) 0.0 [0]
T_melt (K) 873.0 [873]
approx_alpha T [T] F
Anderson-Gruneisen F [F] T
speciation_precision 0.1E-4 [1d-5] <1; absolute
speciation_max_it 100 [100]
GFSM F [F] T GFSM/special_component toggle
hybrid_EoS_H2O 4 [4] 0-2, 4-7
hybrid_EoS_CO2 4 [4] 0-4, 7
hybrid_EoS_CH4 0 [0] 0-1, 7
aq_bad_results err [err] 101 102 103 ignore
aq_lagged_speciation F [F] T
aq_ion_H+ T [T] F => use OH-
aq_oxide_components F [F] T
aq_solvent_solvus T [T] F
aq_vapor_epsilon 1.0 [1.]

Input/Output options:

pause_on_error T [T] F
timing T [T] F
auto_exclude T [T] F

To change these options see: www.perplex.ethz.ch/perplex_options.html

Summary of make-definition entities:

cumm_dqf fo8L q8L cenjh odi qjL dijL fojL foTL mcpv cmpv foHL qHL

Summary of saturated-component entities:

for: SiO2

q trd crst coe stv qL q8L qjL qHL

** Starting auto_refine computational stage **

cycle 1 1 1
cycle 2 2 2
cycle 3 3 3

Initial number of divariant assemblages to be tested is: 3

Testing divariant assemblage 1, 2 assemblages remaining to be tested.

finished with equilibrium (1) ta cc = tr

****warning ver047**** univariant field 2 terminates at an invariant field that could not be located within the tolerance specified in the thermodynamic data file (PTOL= 0.300000E-02).

finished with equilibrium (2) ta dol = tr

finished with equilibrium (2) ta dol = tr

finished with equilibrium (3) dol = ta cc

finished with equilibrium (4) dol = tr cc

finished with equilibrium (5) mag = ta

finished with equilibrium (5) mag = ta

finished with equilibrium (6) dol mag = tr

****warning ver020**** sfol2

finished with equilibrium (7) tr cc = di

****warning ver047**** univariant field 8 terminates at an invariant field that could not be located within the tolerance specified in the thermodynamic data file (PTOL= 0.300000E-02).

finished with equilibrium (8) dol = di

finished with equilibrium (8) dol = di

finished with equilibrium (8) dol = di

finished with equilibrium (9) ta = en

finished with equilibrium (10) mag = en

finished with equilibrium (11) dol en = tr

finished with equilibrium (10) mag = en

finished with equilibrium (10) mag = en

finished with equilibrium (11) dol en = tr

finished with equilibrium (12) tr = di en

finished with equilibrium (8) dol = di

finished with equilibrium (13) ta = anth

finished with equilibrium (14) anth = en

Testing divariant assemblage 2, 2 assemblages remaining to be tested.

finished with equilibrium (7) tr cc = di

Testing divariant assemblage 3, 2 assemblages remaining to be tested.

finished with equilibrium (15) cc = wo

Testing divariant assemblage 4, 2 assemblages remaining to be tested.

Testing divariant assemblage 5, 3 assemblages remaining to be tested.

Testing divariant assemblage 6, 3 assemblages remaining to be tested.

Testing divariant assemblage 7, 2 assemblages remaining to be tested.

Testing divariant assemblage 8, 2 assemblages remaining to be tested.

Testing divariant assemblage 9, 2 assemblages remaining to be tested.

Testing divariant assemblage 10, 3 assemblages remaining to be tested.

Testing divariant assemblage 11, 3 assemblages remaining to be tested.

Testing divariant assemblage 12, 3 assemblages remaining to be tested.

Testing divariant assemblage 13, 3 assemblages remaining to be tested.

Testing divariant assemblage 14, 3 assemblages remaining to be tested.

Testing divariant assemblage 15, 2 assemblages remaining to be tested.

Testing divariant assemblage 16, 2 assemblages remaining to be tested.

Testing divariant assemblage 17, 1 assemblages remaining to be tested.

Testing divariant assemblage	18,	0 assemblages remaining to be tested.
Testing divariant assemblage	19,	1 assemblages remaining to be tested.
Testing divariant assemblage	20,	0 assemblages remaining to be tested.
Testing divariant assemblage	21,	0 assemblages remaining to be tested.
Testing divariant assemblage	22,	0 assemblages remaining to be tested.

(3) Plotting the calculated phase diagram (PSVDRAW)

Run PSVDRAW to plot the calculated phase diagram:

```
C:\PERPLEX\Perplex691>psvdraw
```

Perple_X version 6.9.1, source updated January 3, 2022.

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Enter the project or plot file name [i.e., without the .plt suffix]:

```
ex5_3
```

Perple_X plot options are currently set as:

```
Keyword:      Value:  Permitted values [default]:
axis_label_scale  1.20  [1.2] (rel)
bounding_box :
    0  [0] x-min (pts)
    0  [0] y-min (pts)
    800 [800] x-length (pts)
    800 [800] y-length (pts)
field_fill      T  [T] F
field_label     T  [T] F
numeric_field_label F  [F] T, if T PSSECT writes list to *_assemblages.txt
replicate_label 0.250 0->1 [0.025]
field_label_scale 0.75  [0.72] (rel)
font            Helvetica
grid            F  [F] T
half_ticks      T  [T] F
line_width      1.00  0-99 [1.] (pts)
picture_transformation :
    0.180 [0.18] x-scale (rel)
    0.180 [0.18] y-scale (rel)
    130.  [0.18] x-translation (pts)
    220.  [0.18] y-translation (pts)
    0.00  [0.0] rotation (deg)
plot_aspect_ratio 1.000 [1.0] x_axis_length/y_axis_length
splines          T  [T] F
tenth_ticks      F  [F] T
text_scale       1.000 [1.] (rel)
plot_extra_data
```

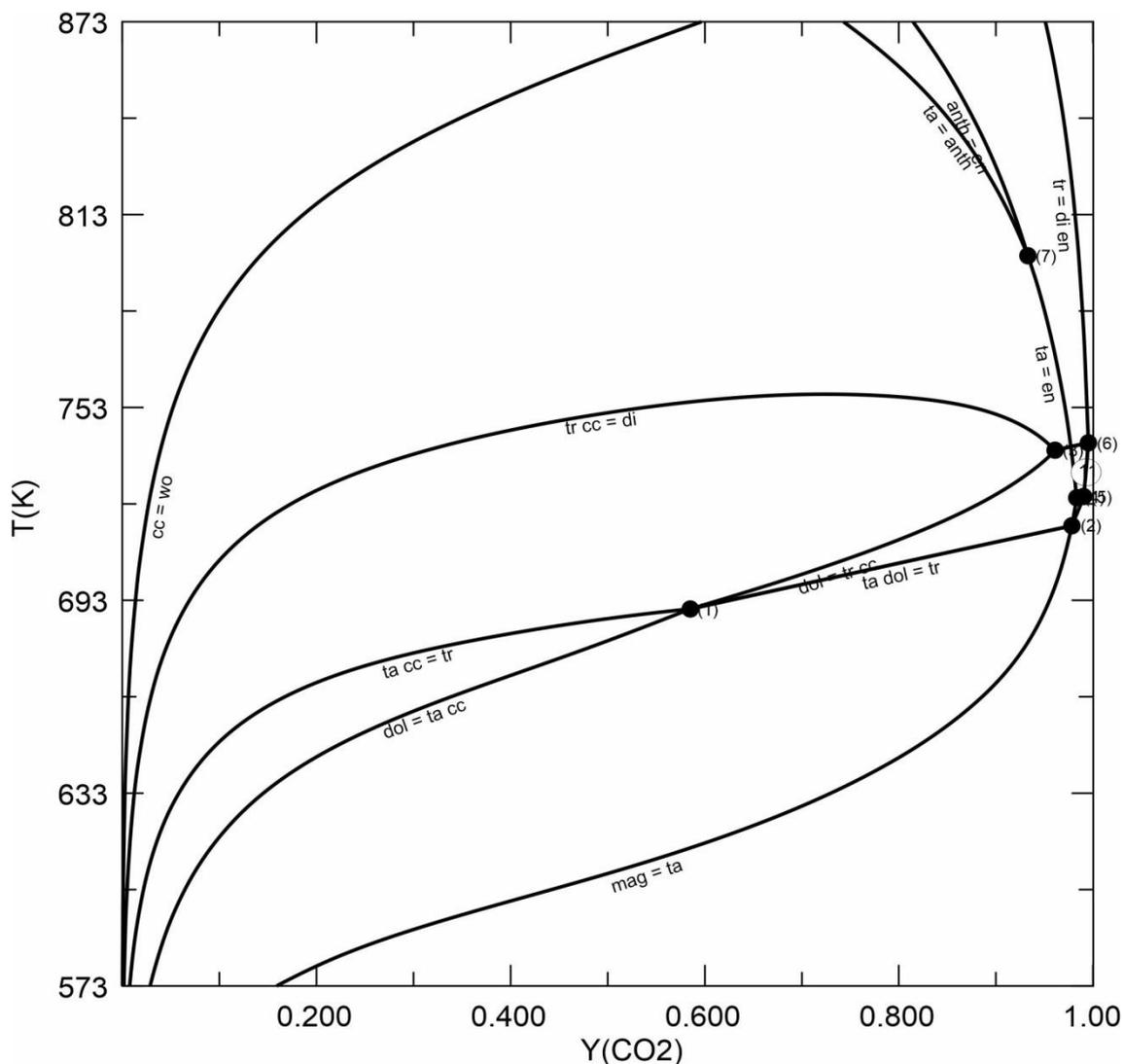
To change these options edit or create the plot option file

See: www.perplex.ethz.ch/perplex_plot_options.html

PostScript will be written to file: ex5_3.ps

Modify the default plot (y/n)?

N



Ex. 5.4 – Isobaric T-XCO₂ pseudosection of a siliceous limestone for the composition 6Qtz–2Dol–1Cal (see Bucher & Grapes, 2011; Fig. 6.12)

(1) Definition of the problem (BUILD)

The problem is the same as in Ex. 5.2, except for the composition of the system that is now 6Qtz + 2Dol + 1Cal, corresponding to 6SiO₂ + 2MgO + 3CaO. You can edit the `ex5_2.dat` input file (change the name in `ex5_4`) (see below).

```
begin thermodynamic component list
MgO 1 2.00000 0.00000 0.00000 molar amount
CaO 1 3.00000 0.00000 0.00000 molar amount
SiO2 1 6.00000 0.00000 0.00000 molar amount
end thermodynamic component list
```

(2) Doing the calculation (VERTEX)

Run VERTEX to make the calculation:

```
C:\PERPLEX\Perplex691>vertex
```

Perple_X version 6.9.1, source updated January 3, 2022.

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Enter the project name (the name assigned in BUILD) [default = my_project]:

```
ex5_4
```

```
Reading problem definition from file: ex5_4.dat
```

```
Reading thermodynamic data from file: hp62ver.dat
```

```
Writing print output to file: ex5_4.plt
```

```
Writing plot output to file: ex5_4.plt
```

```
Writing phase assemblage data to file: ex5_4.blk
```

```
Reading solution models from file: not requested
```

```
Reading Perple_X options from: perplex_option.dat
```

```
Writing seismic data options to: ex5_4_seismic_data.txt
```

```
Writing Perple_X option summary to: not requested
```

Perple_X computational option settings for VERTEX:

Keyword: Value: Permitted values [default]:

Auto-refine options:

auto_refine aut [auto] manual off

replicate_threshold 0.1E-1 [1e-2]; static opt; <0 => no replica test

rep_dynamic_threshold 0.1E-2 [1d-3]; dynamic opt; <0 => no replica test

re-refine F [F] T

intermediate_savrpc F [F] T

intermediate_savdyn F [F] T

keep_all_rpc T [T] F

Free energy minimization options:

MINFRC_diff_increment 0.1E-6 [1e-7] 1e-3 => 1e-9

MINFXC_solver 0 [0] >= 0 - speci2, -1 - MINFXC

optimization_max_it 40 [40] >1

optimization_precision 0.1E-3 [1e-4], 1e-1 => 1e-6, absolute

order_check F [F] T

refinement_points 5 [auto] 1->14

refinement_switch F [T] F

scatter-points T [T] F

scatter-increment 0.1E-1 [1e-2] 1e-2 => 1e-7

solvus_tolerance_ll aut [0.2] 0->1

zero_mode 0.1E-5 [1e-6] 0->1; < 0 => off

2D grid options:

x_nodes 10 / 40 [10/40] >0, <2048; effective x-resolution 10 / 313 nodes

y_nodes 10 / 40 [10/40] >0, <2048; effective y-resolution 10 / 313 nodes

grid_levels 1 / 4 [1/4] >0, <10

linear_model on [on] off

Solution subdivision options:

initial_resolution: 0.2500 [1/4] 0->1; 0 => off
stretch_factor 0.0020 [2d-3] >0
non_linear_switch F [F] T
subdivision_override off [lin] off str
refine_endmembers F [F] T

Thermodynamic options:

solvus_tolerance aut [aut] or 0->1; aut = automatic, 0 => p=c pseudocompounds, 1 => homogenize
T_stop (K) 0.0 [0]
T_melt (K) 873.0 [873]
approx_alpha T [T] F
Anderson-Gruneisen F [F] T
speciation_precision 0.1E-4 [1d-5] <1; absolute
speciation_max_it 100 [100]
GFSM F [F] T GFSM/special_component toggle
hybrid_EoS_H2O 4 [4] 0-2, 4-7
hybrid_EoS_CO2 4 [4] 0-4, 7
hybrid_EoS_CH4 0 [0] 0-1, 7
aq_bad_results err [err] 101 102 103 ignore
aq_lagged_speciation F [F] T
aq_ion_H+ T [T] F => use OH-
aq_oxide_components F [F] T
aq_solvent_solvus T [T] F
aq_vapor_epsilon 1.0 [1.]

Input/Output options:

pause_on_error T [T] F
timing T [T] F
auto_exclude T [T] F
logarithmic_p F [F] T
bad_number NaN [NaN]
interim_results aut [auto] off manual

Information file output options:

option_list_files F [F] T; echo computational options
pseudocompound_file F [F] T; echo static pseudocompound compositions
auto_refine_file F [T] F; echo auto-refine compositions
seismic_data_file T [F] T; echo seismic wavespeed options

To change these options see: www.perplex.ethz.ch/perplex_options.html

Summary of make-definition entities:

cumm_dqf fo8L q8L cenjh odi qjL dijL fojL foTL mcpv cmpv foHL qHL

warning ver099 no data for aqueous species, aq_output and aq_lagged_speciation disabled.

** Starting exploratory computational stage **

2.5% done with low level grid.
5.0% done with low level grid.
7.5% done with low level grid.
10.0% done with low level grid.
12.5% done with low level grid.
15.0% done with low level grid.
17.5% done with low level grid.

20.0% done with low level grid.
22.5% done with low level grid.
25.0% done with low level grid.
27.5% done with low level grid.
30.0% done with low level grid.
32.5% done with low level grid.
35.0% done with low level grid.
37.5% done with low level grid.
40.0% done with low level grid.
42.5% done with low level grid.
45.0% done with low level grid.
47.5% done with low level grid.
50.0% done with low level grid.
52.5% done with low level grid.
55.0% done with low level grid.
57.5% done with low level grid.
60.0% done with low level grid.
62.5% done with low level grid.
65.0% done with low level grid.
67.5% done with low level grid.
70.0% done with low level grid.
72.5% done with low level grid.
75.0% done with low level grid.
77.5% done with low level grid.
80.0% done with low level grid.
82.5% done with low level grid.
85.0% done with low level grid.
87.5% done with low level grid.
90.0% done with low level grid.
92.5% done with low level grid.
95.0% done with low level grid.
97.5% done with low level grid.
100.0% done with low level grid.

Beginning grid refinement stage.

204 grid cells to be refined at grid level 2

refinement at level 2 involved 436 minimizations

2036 minimizations required of the theoretical limit of 6241

366 grid cells to be refined at grid level 3

...working (66 minimizations done)

...working (567 minimizations done)

refinement at level 3 involved 705 minimizations

2741 minimizations required of the theoretical limit of 24649

682 grid cells to be refined at grid level 4

...working (363 minimizations done)

...working (864 minimizations done)

refinement at level 4 involved 1270 minimizations

4011 minimizations required of the theoretical limit of 98596

Exploratory stage generated:

Total number of compositions: 0

** Starting auto-refine computational stage **

2.5% done with low level grid.
5.0% done with low level grid.
7.5% done with low level grid.
10.0% done with low level grid.
12.5% done with low level grid.
15.0% done with low level grid.
17.5% done with low level grid.
20.0% done with low level grid.
22.5% done with low level grid.
25.0% done with low level grid.
27.5% done with low level grid.
30.0% done with low level grid.
32.5% done with low level grid.
35.0% done with low level grid.
37.5% done with low level grid.
40.0% done with low level grid.
42.5% done with low level grid.
45.0% done with low level grid.
47.5% done with low level grid.
50.0% done with low level grid.
52.5% done with low level grid.
55.0% done with low level grid.
57.5% done with low level grid.
60.0% done with low level grid.
62.5% done with low level grid.
65.0% done with low level grid.
67.5% done with low level grid.
70.0% done with low level grid.
72.5% done with low level grid.
75.0% done with low level grid.
77.5% done with low level grid.
80.0% done with low level grid.
82.5% done with low level grid.
85.0% done with low level grid.
87.5% done with low level grid.
90.0% done with low level grid.
92.5% done with low level grid.
95.0% done with low level grid.
97.5% done with low level grid.
100.0% done with low level grid.

Beginning grid refinement stage.

204 grid cells to be refined at grid level 2
refinement at level 2 involved 436 minimizations
2036 minimizations required of the theoretical limit of 6241
366 grid cells to be refined at grid level 3
...working (66 minimizations done)
...working (567 minimizations done)
refinement at level 3 involved 705 minimizations

2741 minimizations required of the theoretical limit of 24649
 682 grid cells to be refined at grid level 4
 ...working (363 minimizations done)
 ...working (864 minimizations done)
 refinement at level 4 involved 1270 minimizations
 4011 minimizations required of the theoretical limit of 98596

Timing	min.	% of total
Static G calculation	0.20833E-02	9.8
Dynamic G calculation	0.0000	0.0
Static LP	0.52083E-03	2.4
Dynamic LP	0.0000	0.0
Successive QP	0.0000	0.0
Total of above	0.26042E-02	12.2
Total elapsed time	0.21354E-01	100.0

End of job: ex5_4

(3) Plotting the calculated phase diagram (PSSECT)

Run PSSECT to plot the calculated pseudosection:

C:\PERPLEX\Perplex691>pssect

Perple_X version 6.9.1, source updated January 3, 2022.

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Enter the project name (the name assigned in BUILD) [default = my_project]:

ex5_4

Reading Perple_X options from: perplex_option.dat

Perple_X plot options are currently set as:

```

Keyword:      Value:  Permitted values [default]:
axis_label_scale  1.20  [1.2] (rel)
bounding_box :
      0  [0] x-min (pts)
      0  [0] y-min (pts)
      800 [800] x-length (pts)
      800 [800] y-length (pts)
field_fill      T  [T] F
field_label     T  [T] F
numeric_field_label  F  [F] T, if T PSSECT writes list to *_assemblages.txt
replicate_label  0.250  0->1 [0.025]
field_label_scale  0.75  [0.72] (rel)
font            Helvetica
grid           F  [F] T
half_ticks     T  [T] F
line_width     1.00  0-99 [1.] (pts)

```

```

picture_transformation :
    0.180 [0.18] x-scale (rel)
    0.180 [0.18] y-scale (rel)
    130. [0.18] x-translation (pts)
    220. [0.18] y-translation (pts)
    0.00 [0.0] rotation (deg)
plot_aspect_ratio 1.000 [1.0] x_axis_length/y_axis_length
splines          T      [T] F
tenth_ticks      F      [F] T
text_scale       1.000 [1.] (rel)
plot_extra_data

```

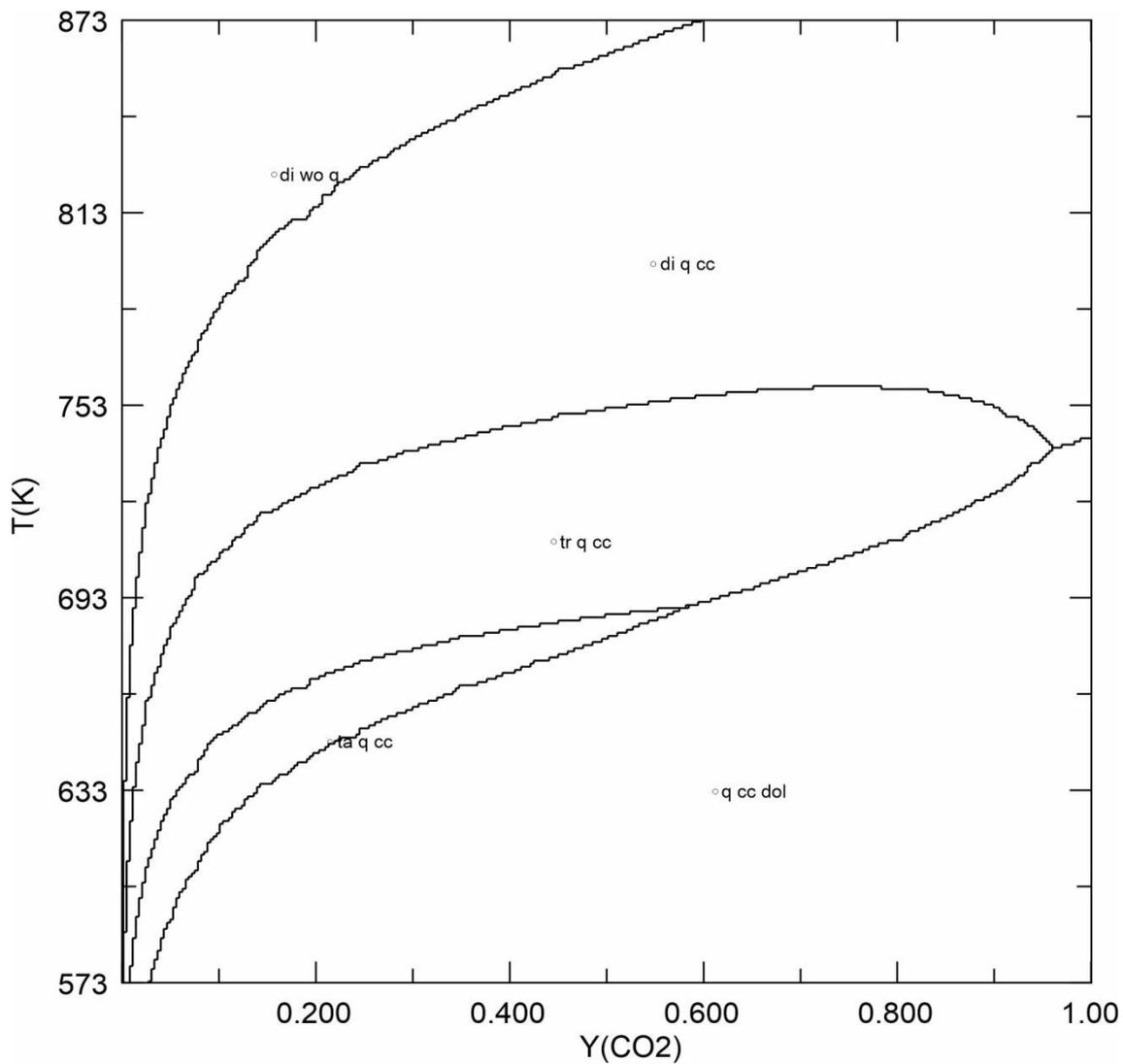
To change these options edit or create the plot option file

See: www.perplex.ethz.ch/perplex_plot_options.html

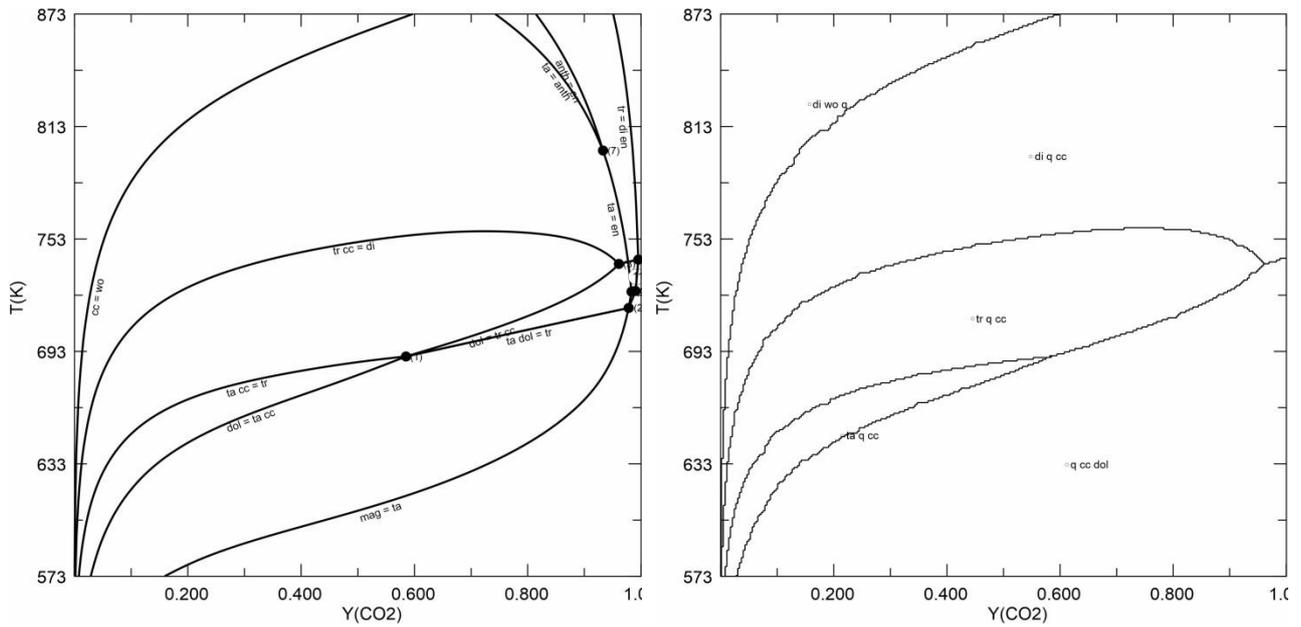
PostScript will be written to file: ex5_4.ps

Modify the default plot (y/n)?

N



Comparison between projections and pseudosections



Comparison between the isobaric T-X(CO₂) projection for a generic siliceous limestone containing excess quartz (Ex. 5.3) and the pseudosection calculated for a bulk composition MgO=2, CaO=3, SiO₂=6 mol% (6Qtz+2Dol+1Cal; Ex. 5.4). **This specific bulk composition “sees” (i.e. is sensible to) only some of the reactions predicted by the P-T projection.**

Ex 6

Ex. 6 – T-XMg section for the CaCO_3 - MgCO_3 system (*sol/vus* relations)

This exercise explains how to calculate *sol/vus* relations in the system CaCO_3 - MgCO_3 . In this system two miscibility gaps exist, and the phases on either side of the gaps are calcite/dolomite, and dolomite/magnesite, respectively. The amounts of MgCO_3 in calcite in equilibrium with dolomite, and that of CaCO_3 in magnesite in equilibrium with dolomite, change as a function of temperature, and can be used as geothermometers. The effect of pressure on the Cal-Dol and Dol-Mag *sol/vi* is investigated by calculating the same phase diagram at different pressures.

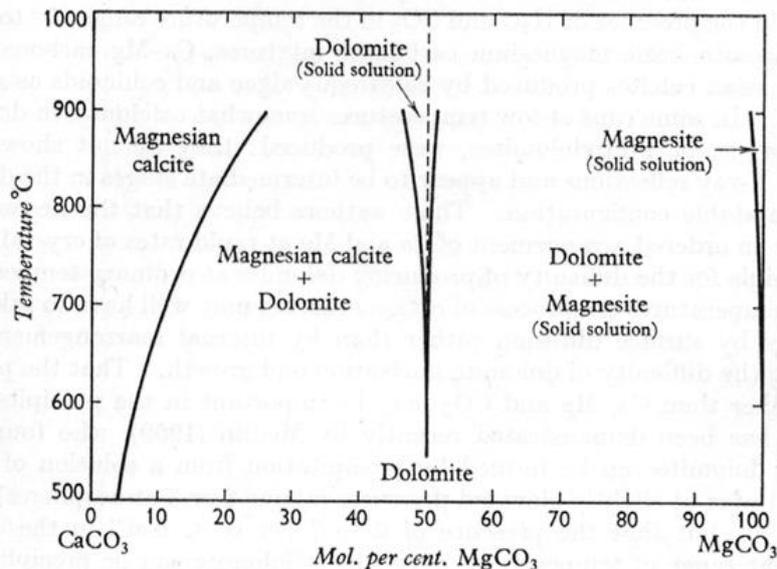


FIG. 53. The CaCO_3 - MgCO_3 system, at CO_2 pressures sufficient to prevent decomposition of the carbonates (after Goldsmith, 1959).

The issue can be treated as a simple isobaric T-X pseudosection, where X (XMg) varies between 0 (XMg=0; Cal) and 1 (XMg=1; Mag). Opposite to Ex. 4 and 5, **SOLID SOLUTIONS MUST NOW BE CONSIDERED**. Perplex deals with solid solutions by creating a whole set of “pseudocompounds” (intermediate compositions), and treating each of them like a separate phase. Thus, if a carbonate with composition Ca_{90} has a lower free energy than Ca_{95} at a particular P-T condition, Ca_{90} will be considered as the stable carbonate.

Pseudocompounds are indicated with abbreviations, whose meaning is sometimes not immediately understandable. To understand the meaning of these abbreviations, I suggest changing to T (true) the default value of the pseudocompound_file keyword in the perplex_option.dat file. Doing in this way, VERTEX will create an additional output file, listing the composition of each pseudocompound.

(1) Definition of the problem (BUILD)

```
C:\PERPLEX\Perplex691>build
```

Perple_X version 6.9.1, source updated January 3, 2022.

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NO is the default (blank) answer to all Y/N prompts

Enter a name for this project (the name will be used as the root for all output file names) [default = my_project]:

ex6_5kbar

The problem definition file will be named: ex6_5kbar.dat

Enter thermodynamic data file name [default = hp02ver.dat]:

hp62ver.dat

Enter the computational option file name [default = perplex_option.dat]:

See: www.perplex.ethz.ch/perplex_options.html

Reading Perple_X options from: perplex_option.dat

The current data base components are:

Na2O MgO Al2O3 SiO2 K2O CaO TiO2 MnO FeO NiO ZrO2 Cl2 O2 H2O CO2 CuO Cr2O3 S2 F2 N2 ZnO

Transform them (Y/N)?

n

Specify computational mode:

- 1 - Convex-Hull minimization
- 2 - Constrained minimization on a 2d grid [default]
- 3 - Constrained minimization on a 1d grid
- 4 - Output pseudocompound data
- 5 - 1-d Phase fractionation
- 6 - 0-d Infiltration-reaction-fractionation
- 7 - 2-d Phase fractionation (FRAC2D and TITRATE reactive transport models)

Use Convex-Hull minimization for Schreinemakers projections or phase diagrams with > 2 independent variables. Use constrained minimization for phase diagrams or phase diagram sections with < 3 independent variables.

The problem can be treated as an isobaric T-X pseudosection, where X varies between 0 (XMg=0; Cal) and 1 (XMg=1; Mag).

2

Calculations with a saturated fluid (Y/N)?

y

Select the independent saturated fluid components:

H2O CO2

Enter names, 1 per line, press <enter> to finish:

For C-O-H fluids it is only necessary to select volatile species present in the solids of interest. If the species listed here are H2O and CO2, then to constrain O2 chemical potential to be consistent with C-O-H fluid speciation treat O2 as a saturated component. Refer to the Perple_X Tutorial for details.

CO2

Calculations with saturated components (Y/N)?

n

Use chemical potentials, activities or fugacities as independent variables (Y/N)?

n

Select thermodynamic components from the set:

Na2O MgO Al2O3 SiO2 K2O CaO TiO2 MnO FeO NiO ZrO2 Cl2 O2 H2O CuO Cr2O3 S2 F2 N2 ZnO

Enter names, 1 per line, press <enter> to finish:

MgO

CaO

Because the thermodynamic data file identifies: CO2 as special components, you will be prompted next for the EoS to be used for the corresponding components and mixtures thereof. To override this behavior, e.g., to use a generic hybrid fluid EoS, delete the special_component section from the thermodynamic data file header.

NOTE: the EoS choice specified here will override the EoS choice specified by the hybrid_EoS option, to override this behavior delete the special_component section from the the thermodynamic data file header.

Select fluid equation of state:

- 0 - X(CO2) H2O-CO2 Modified Redlich-Kwong (MRK) DeSantis et al 74
- 1 - X(CO2) H2O-CO2 HSMRK Kerrick & Jacobs 81
- 2 - X(CO2) H2O-CO2 MRK hybrid-EoS*
- 5 - X(CO2) H2O-CO2 CORK Holland & Powell 91, 98
- 8 - f(O2/CO2) C-buffered COH MRK hybrid-EoS*
- 10 - X(O) C-buffered COH MRK hybrid-EoS Connolly & Cesare 93*
- 12 - X(O)-f(S2) C-buffered COHS MRK hybrid-EoS Connolly & Cesare 93*
- 13 - X(H2) H2O-H2 MRK hybrid-EoS*
- 14 - X(CO2) H2O-CO2 Pitzer & Sterner 94; Holland & Powell mixing 03
- 15 - X(H2) H2O-H2 low T MRK hybrid-EoS*
- 16 - X(O) H-O MRK hybrid-EoS*
- 17 - X(O)-f(S2) H-O-S MRK hybrid-EoS*
- 19 - X(O)-X(S) C-buffered COHS MRK hybrid-EoS Connolly & Cesare 93*
- 20 - X(O)-X(C) COHS MRK hybrid-EoS Connolly & Cesare 93*
- 24 - f(O2/CO2)-N/C C-buffered COHN MRK hybrid-EoS*
- 25 - X(CO2)-X(NaCl) H2O-CO2-NaCl Aranovich et al 10
- 26 - X(O) O-Si MRK Connolly 16
- 27 - X(O)-X(C) C-O-H MRK hybrid-EoS*

*Hybrid EoS use the following pure species EoS, to change these associations modify the hybrid_EoS keywords in the perplex_option file:

- H2O - PSEoS Pitzer & Sterner 1994
- CO2 - PSEoS Pitzer & Sterner 1994
- CH4 - MRK DeSantis et al 1974

5

The data base has P(bar) and T(K) as default independent potentials.

Make one dependent on the other, e.g., as along a geothermal gradient (y/n)?

n

Select x-axis variable:

- 1 - P(bar)

2 - T(K)

3 - Y(CO2)

4 - Composition X_C1* (user defined)

*Although only one component is specified for the Y(CO2) phase, its equation of state permits use of its compositional variable:

*X_C1 can not be selected as the y-axis variable

4

Select y-axis variable:

1 - P(bar)

2 - T(K)

3 - Y(CO2)

2

Enter minimum and maximum values, respectively, for: T(K)

573

1273

Specify sectioning value for: P(bar)

5000

Specify sectioning value for: Y(CO2)

The fluid is pure CO2.

1

For gridded minimization, grid resolution is determined by the number of levels (grid_levels) and the resolution at the lowest level in the X- and Y-directions (x_nodes and y_nodes) these parameters are currently set for the exploratory and autorefine cycles as follows:

stage grid_levels xnodes ynodes effective resolution

exploratory 1 10 10 10 x 10 nodes

auto-refine 4 40 40 313 x 313 nodes

To change these options edit or create the file perplex_option.dat

See: www.perplex.ethz.ch/perplex_options.html#grid_parameters

Specify component amounts by mass (Y/N)?

n

The amounts you enter next need not be normalized; regardless of units, they define the molar amount of the system

The bulk composition of the system will be computed as:

$$C = C0*(1 - X_C1) + C1*X_C1$$

where X_C1 varies between 0 and 1, and C0 and C1 are the compositions specified next.

To compute bulk compositions as: $C = C0 + C1*X_C1$

change the computational option keyword closed_c_space.

Enter the molar amounts of the components:

MgO CaO

to define the composition C0

Composition C0 should be CaCO3, therefore it is defined as CaO=1, MgO=0

0

1

Enter the molar amounts of the components:

MgO CaO

to define the composition C1

Composition C1 should be MgCO₃, therefore it is defined as CaO=0, MgO=1

1

0

Output a print file (Y/N)?

y

Exclude pure and/or endmember phases (Y/N)?

y

Do you want to be prompted for phases (Y/N)?

n

Enter names, 1 per line, press <enter> to finish:

per

per

dol

See below the reason why the dol end-member is excluded from the calculation.

Include solution models (Y/N)?

Y

Enter the solution model file name [default = solution_model.dat]:

[enter]

...

Select models from the following list, enter 1 per line, press <enter> to finish

carbonate models: Do(AE) Cc(AE) oCcM(HP) Carb(M) oCcM(EF) dis(EF)

fluid models: COH-Fluid COH-Fluid+

For details on these models see: www.perplex.ethz.ch/perplex_solution_model_glossary.html

or read the commentary in the solution model file.

Do(AE)

Cc(AE)

Do(AE) and Cc(AE) are the solution models for dolomite and magnesite from Anovitz & Essene (1987), respectively. Cc(AE) also models Mg-calcite.

"The Do(AE) model requires fictive do-structure endmembers that have a standard state $G_{20920j} >$ than the Cal-structure endmember, these are made here by a "DQF" correction." This "warning" (see [solution_model.dat](#) file) implies that the dol end-member must be excluded from the calculation.

Enter calculation title:

Ex6_5kbar

(2) Doing the calculation (VERTEX)

Run VERTEX to make the calculation:

C:\PERPLEX\Perplex691>vertex

Perple_X version 6.9.1, source updated January 3, 2022.

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Enter the project name (the name assigned in BUILD) [default = my_project]:

ex6_5kbar

Reading problem definition from file: ex6_5kbar.dat

Reading thermodynamic data from file: hp62ver.dat

Writing print output to file: ex6_5kbar.plt

Writing plot output to file: ex6_5kbar.plt

Writing phase assemblage data to file: ex6_5kbar.blk

Reading solution models from file: solution_model.dat

Reading Perple_X options from: perplex_option.dat

Writing auto refine summary to: not requested

Writing seismic data options to: ex6_5kbar_seismic_data.txt

Writing pseudocompound glossary to: ex6_5kbar_pseudocompound_glossary.txt

Writing Perple_X option summary to: not requested

Perple_X computational option settings for VERTEX:

Keyword: Value: Permitted values [default]:

Auto-refine options:

auto_refine aut [auto] manual off

replicate_threshold 0.1E-1 [1e-2]; static opt; <0 => no replica test

rep_dynamic_threshold 0.1E-2 [1d-3]; dynamic opt; <0 => no replica test

re-refine F [F] T

intermediate_savrpc F [F] T

intermediate_savdyn F [F] T

keep_all_rpc T [T] F

Free energy minimization options:

MINFRC_diff_increment 0.1E-6 [1e-7] 1e-3 => 1e-9

MINFXC_solver 0 [0] >= 0 - speci2, -1 - MINFXC

optimization_max_it 40 [40] >1

optimization_precision 0.1E-3 [1e-4], 1e-1 => 1e-6, absolute

order_check F [F] T

refinement_points 4 [auto] 1->14

refinement_switch F [T] F

scatter-points T [T] F

scatter-increment 0.1E-1 [1e-2] 1e-2 => 1e-7

solvus_tolerance_ll aut [0.2] 0->1

zero_mode 0.1E-5 [1e-6] 0->1; < 0 => off

2D grid options:

x_nodes 10 / 40 [10/40] >0, <2048; effective x-resolution 10 / 313 nodes

y_nodes 10 / 40 [10/40] >0, <2048; effective y-resolution 10 / 313 nodes

grid_levels 1 / 4 [1/4] >0, <10

linear_model on [on] off

Composition options:

closedc_space T [T] F

Solution subdivision options:

initial_resolution: 0.2500 [1/4] 0->1; 0 => off

stretch_factor 0.0020 [2d-3] >0
non_linear_switch F [F] T
subdivision_override off [lin] off str
refine_endmembers F [F] T

Thermodynamic options:

solvus_tolerance aut [aut] or 0->1; aut = automatic, 0 => p=c pseudocompounds, 1 => homogenize
T_stop (K) 0.0 [0]
T_melt (K) 873.0 [873]
approx_alpha T [T] F
Anderson-Gruneisen F [F] T
speciation_precision 0.1E-4 [1d-5] <1; absolute
speciation_max_it 100 [100]
GFSM F [F] T GFSM/special_component toggle
hybrid_EoS_H2O 4 [4] 0-2, 4-7
hybrid_EoS_CO2 4 [4] 0-4, 7
hybrid_EoS_CH4 0 [0] 0-1, 7
aq_bad_results err [err] 101 102 103 ignore
aq_lagged_speciation F [F] T
aq_ion_H+ T [T] F => use OH-
aq_oxide_components F [F] T
aq_solvent_solvus T [T] F
aq_vapor_epsilon 1.0 [1.]

Input/Output options:

pause_on_error T [T] F
timing T [T] F
auto_exclude T [T] F
logarithmic_p F [F] T
bad_number NaN [NaN]
interim_results aut [auto] off manual

Information file output options:

option_list_files F [F] T; echo computational options
pseudocompound_file T [F] T; echo static pseudocompound compositions
auto_refine_file F [T] F; echo auto-refine compositions
seismic_data_file T [F] T; echo seismic wavespeed options

To change these options see: www.perplex.ethz.ch/perplex_options.html

****warning ver099**** no data for aqueous species, aq_output and aq_lagged_speciation disabled.

Solution model summary:

****warning ver114**** the following endmembers are missing for Do(AE)
sid

3 pseudocompounds generated for: Do(AE)

****warning ver114**** the following endmembers are missing for Cc(AE)
sid

3 pseudocompounds generated for: Cc(AE)

Total number of pseudocompounds: 6

Summary of included solution models:

Do(AE) Cc(AE)

This section shows the total number of pseudocompounds considered by VERTEX; the number of pseudocompounds is controlled by some of the perplex_option keywords. **The highest is the number of pseudocompounds, the longest is the calculation (and the virtual memory consumed).**

For pseudosection calculations (involving solid solutions), VERTEX divides the calculation in two stages. The **EXPLORATORY STAGE** is used to roughly establish the stable solution compositions; in the **AUTO-REFINE STAGE**, VERTEX refines the previous calculation by:

- 1) Eliminating solutions that were not stable in the exploratory calculation.
- 2) Restricting compositional ranges of solutions to the ranges established in the exploratory calculation
- 3) Increasing resolution of compositions within these restricted ranges.

This is the beginning of EXPLORATORY STAGE

** Starting exploratory computational stage **

9.1% done with low level grid.
18.2% done with low level grid.
27.3% done with low level grid.
36.4% done with low level grid.
45.5% done with low level grid.
54.5% done with low level grid.
63.6% done with low level grid.
72.7% done with low level grid.
81.8% done with low level grid.
90.9% done with low level grid.

Exploratory stage generated:

12 compositions for: Do(AE)
24 compositions for: Cc(AE)

Total number of compositions: 36

This is the beginning of the AUTO-REFINE STAGE

** Starting auto_refine computational stage **

2.5% done with low level grid.
5.0% done with low level grid.
7.5% done with low level grid.
10.0% done with low level grid.
12.5% done with low level grid.
15.0% done with low level grid.
17.5% done with low level grid.
20.0% done with low level grid.
22.5% done with low level grid.
25.0% done with low level grid.
27.5% done with low level grid.
30.0% done with low level grid.
32.5% done with low level grid.
35.0% done with low level grid.
37.5% done with low level grid.
40.0% done with low level grid.
42.5% done with low level grid.

45.0% done with low level grid.
 47.5% done with low level grid.
 50.0% done with low level grid.
 52.5% done with low level grid.
 55.0% done with low level grid.
 57.5% done with low level grid.
 60.0% done with low level grid.
 62.5% done with low level grid.
 65.0% done with low level grid.
 67.5% done with low level grid.
 70.0% done with low level grid.
 72.5% done with low level grid.
 75.0% done with low level grid.
 77.5% done with low level grid.
 80.0% done with low level grid.
 82.5% done with low level grid.
 85.0% done with low level grid.
 87.5% done with low level grid.
 90.0% done with low level grid.
 92.5% done with low level grid.
 95.0% done with low level grid.
 97.5% done with low level grid.
 100.0% done with low level grid.

Beginning grid refinement stage.

164 grid cells to be refined at grid level 2
 refinement at level 2 involved 347 minimizations
 1947 minimizations required of the theoretical limit of 6241
 316 grid cells to be refined at grid level 3
 ...working (154 minimizations done)
 refinement at level 3 involved 621 minimizations
 2568 minimizations required of the theoretical limit of 24649
 620 grid cells to be refined at grid level 4
 ...working (34 minimizations done)
 ...working (535 minimizations done)
 ...working (1036 minimizations done)
 refinement at level 4 involved 1210 minimizations
 3778 minimizations required of the theoretical limit of 98596

Timing	min.	% of total
Static G calculation	0.52083E-03	1.1
Dynamic G calculation	0.88542E-02	19.4
Static LP	0.52083E-03	1.1
Dynamic LP	0.26042E-02	5.7
Successive QP	0.16406E-01	36.0
Total of above	0.28906E-01	63.4
Total elapsed time	0.45573E-01	100.0

End of job: ex6_5kbar

Before plotting the calculated diagram, have a look to the new pseudocompound_file.txt generated by VERTEX. It contains the list of the pseudocompounds with their composition.

(3) Plotting the calculated phase diagram (PSSECT)

Run PSSECT to plot the calculated pseudosection:

```
C:\PERPLEX\Perplex691>pssect
```

Perple_X version 6.9.1, source updated January 3, 2022.

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Enter the project name (the name assigned in BUILD) [default = my_project]:

```
ex6_5kbar
```

Reading Perple_X options from: perplex_option.dat

Perple_X plot options are currently set as:

Keyword:	Value:	Permitted values [default]:
axis_label_scale	1.20	[1.2] (rel)
bounding_box :		
	0	[0] x-min (pts)
	0	[0] y-min (pts)
	800	[800] x-length (pts)
	800	[800] y-length (pts)
field_fill	T	[T] F
field_label	T	[T] F
numeric_field_label	F	[F] T, if T PSSECT writes list to *_assemblages.txt
replicate_label	0.250	0->1 [0.025]
field_label_scale	0.75	[0.72] (rel)
font	Helvetica	
grid	F	[F] T
half_ticks	T	[T] F
line_width	1.00	0-99 [1.] (pts)
picture_transformation :		
	0.180	[0.18] x-scale (rel)
	0.180	[0.18] y-scale (rel)
	130.	[0.18] x-translation (pts)
	220.	[0.18] y-translation (pts)
	0.00	[0.0] rotation (deg)
plot_aspect_ratio	1.000	[1.0] x_axis_length/y_axis_length
splines	T	[T] F
tenth_ticks	F	[F] T
text_scale	1.000	[1.] (rel)
plot_extra_data		

To change these options edit or create the plot option file

See: www.perplex.ethz.ch/perplex_plot_options.html

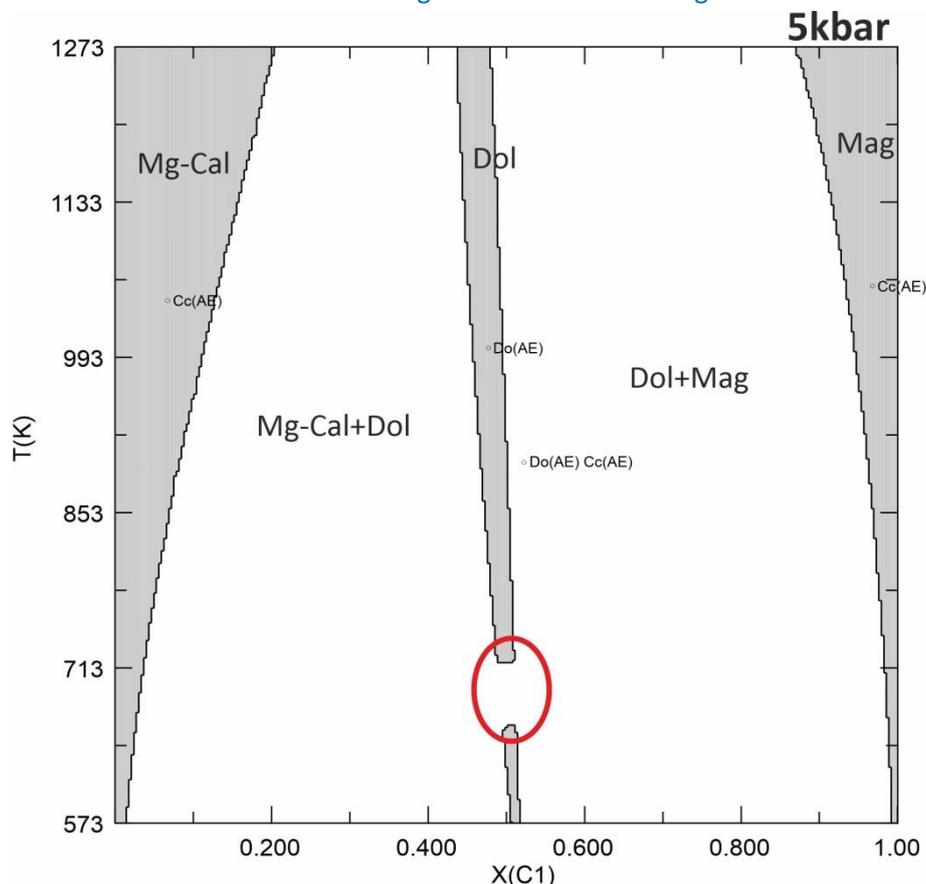
PostScript will be written to file: ex6_5kbar.ps

Modify the default plot (y/n)?

n

There are 2 fields for: Cc(AE)

Because the Cc(AE) solution model treats simultaneously both the Mg-calcite and magnesite solid solutions, they are indicated with the same name on the diagram. Be careful to assign the correct name to each phase.



In the resulting diagram there are two different types of fields: white fields contain two phases (these are the miscibility gaps), whereas grey fields contain one phase.

The red ellipse highlights a “bug”, which can be eliminated by increasing the resolution of the x-y grid used by VERTEX during the gridded minimization calculation.

(4) Increasing the resolution of the x-y grid

For gridded minimization, VERTEX uses a multilevel grid refinement strategy in which phase relations are mapped on an initial grid of resolution $x_nodes * y_nodes$. This grid is refined a number of times equal to $(grid_levels - 1)$ by bisection (Connolly 2005). The x_nodes , y_nodes , $grid_levels$ parameters are set by keywords of the same name in the `perplex_option` file. Each keyword takes two integer values. The first value is used for the exploratory stage of gridded minimization calculations, while the second value is used for the auto-refine stage.

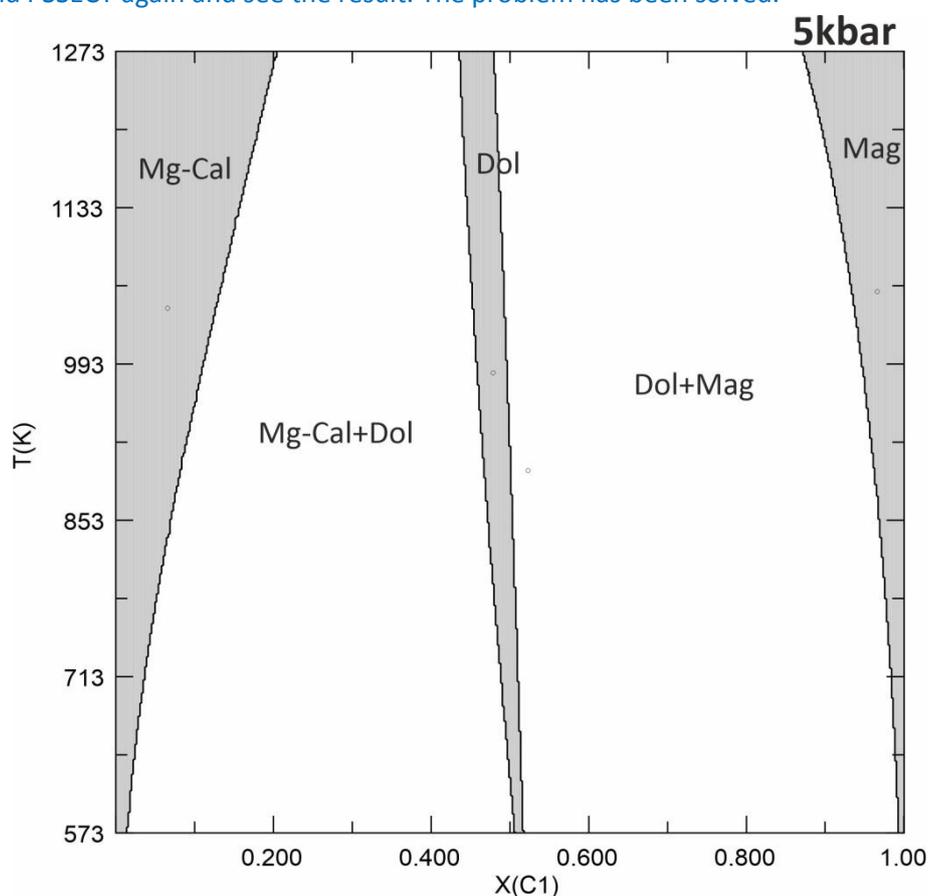
There is no simple rule for the best choices for x_nodes or y_nodes as they depend on the scale of the diagram and the heterogeneity of its phase fields, the default values are 40 and 40 for exploratory and auto-

refinement stages of a calculation. The default values of `grid_levels` are 1 and 4 for exploratory and auto-refinement stages.

Increase the resolution of the grid, by increasing the number of x-y nodes for the auto-refinement stage of calculation from 40 to 60 (open the `perplex_option.dat` file and modify the default value of the `x_nodes` and `y_nodes` parameters).

`x_nodes` 40 60 | [40 40] exploratory and auto-refine (grid parameters keyword group), lowest-level x grid resolution
`y_nodes` 40 60 | [40 40] exploratory and auto-refine (grid parameters keyword group), lowest-level y grid resolution

Run VERTEX and PSSECT again and see the result. The problem has been solved.

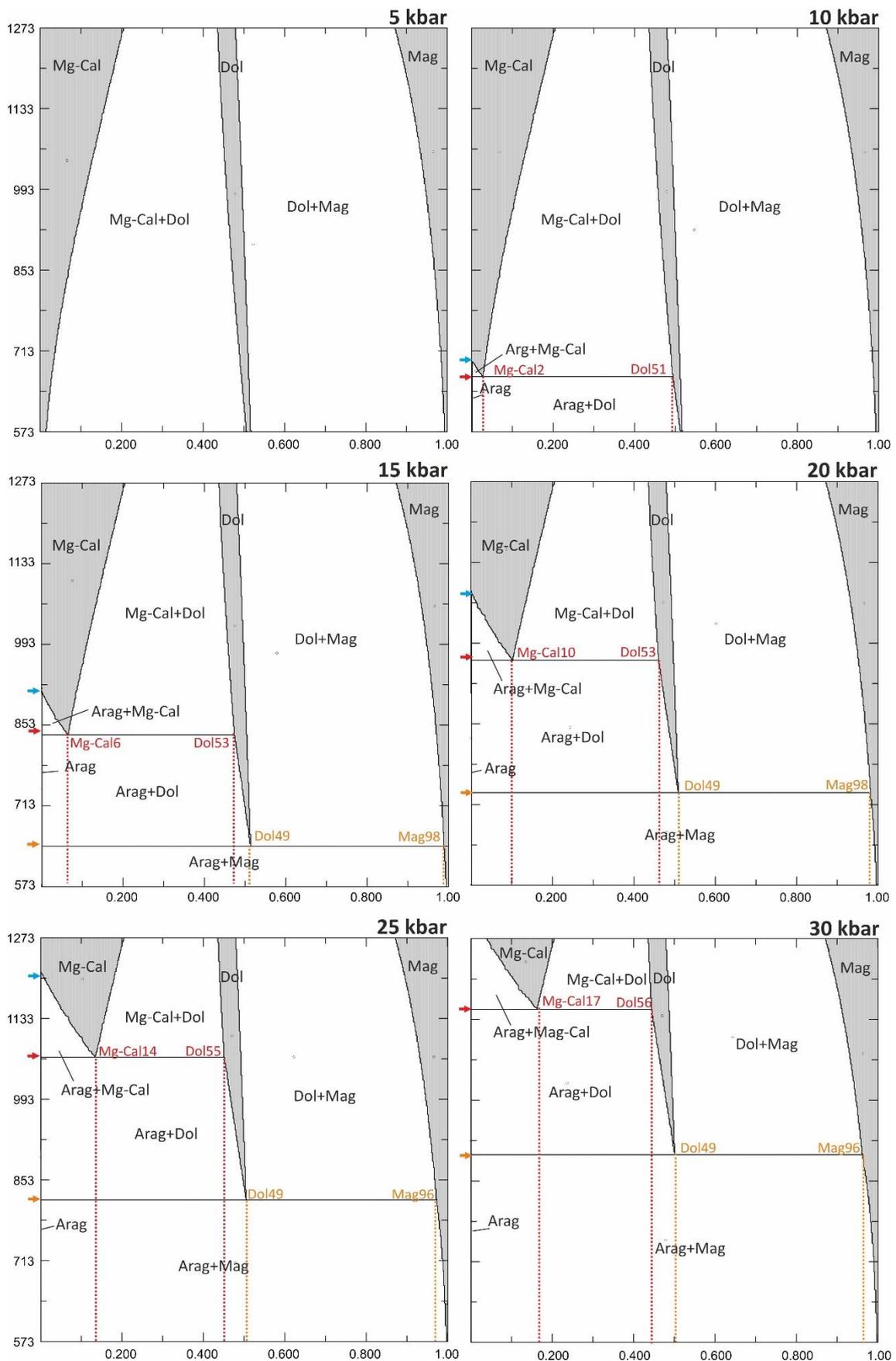


(5) Exploring the influence of pressure on the Cal-Dol and Dol-Mag *solvi*

The influence of pressure on the Cal-Dol and Dol-Mag *solvi* can be investigated by calculating the same phase diagram at different pressures (5 to 30 kbar, every 5 kbar). You can **edit the input file**, by specifying a different pressure (**remember to rename the file**). Pressure is reported at the end of the input file:

```
5000.00 1273.00 1.00000 0.00000 0.00000 max p, t, xco2, u1, u2
5000.00 573.000 1.00000 0.00000 0.00000 min p, t, xco2, u1, u2
0.00000 0.00000 0.00000 0.00000 0.00000 unused place holder post 06
```

Run again VERTEX and PSECT for calculation at 10, 15, 20, 25 and 30 kbar, respectively.



**What happens at the T (and P) conditions indicated by the blue, red and orange arrows?
How many phases are stable at those P-T conditions?**

Ex 7

Ex. 7 – P-T projection for the CaCO₃-MgCO₃ system using solid solutions

This exercise explains how to calculate a P-T projection for the CaCO₃-MgCO₃ system, using solid solutions (rather than end members only).

Combined with Ex. 6, this exercise provides the opportunity for understanding the relationships between isobaric T-X sections and P-T projections.

(1) Definition of the problem (BUILD)

```
C:\PERPLEX\Perplex691>build
```

Perple_X version 6.9.1, source updated January 3, 2022.

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NO is the default (blank) answer to all Y/N prompts

Enter a name for this project (the name will be used as the root for all output file names) [default = my_project]:

```
ex7
```

The problem definition file will be named: ex7.dat

Enter thermodynamic data file name [default = hp02ver.dat]:

```
hp62ver.dat
```

Enter the computational option file name [default = perplex_option.dat]:

See: www.perplex.ethz.ch/perplex_options.html

```
enter
```

Reading Perple_X options from: perplex_option.dat

The current data base components are:

Na2O MgO Al2O3 SiO2 K2O CaO TiO2 MnO FeO NiO ZrO2 Cl2 O2 H2O CO2 CuO Cr2O3 S2 F2 N2 ZnO

Transform them (Y/N)?

```
n
```

Specify computational mode:

- 1 - Convex-Hull minimization
- 2 - Constrained minimization on a 2d grid [default]
- 3 - Constrained minimization on a 1d grid
- 4 - Output pseudocompound data
- 5 - 1-d Phase fractionation
- 6 - 0-d Infiltration-reaction-fractionation
- 7 - 2-d Phase fractionation (FRAC2D and TITRATE reactive transport models)

Use Convex-Hull minimization for Schreinemakers projections or phase diagrams with > 2 independent variables. Use constrained minimization for phase diagrams or phase diagram sections with < 3 independent variables.

1

Calculations with a saturated fluid (Y/N)?

y

Select the independent saturated fluid components:

H2O CO2

Enter names, 1 per line, press <enter> to finish:

For C-O-H fluids it is only necessary to select volatile species present in the solids of interest. If the species listed here are H2O and CO2, then to constrain O2 chemical potential to be consistent with C-O-H fluid speciation treat O2 as a saturated component. Refer to the Perple_X Tutorial for details.

CO2

Calculations with saturated components (Y/N)?

n

Use chemical potentials, activities or fugacities as independent variables (Y/N)?

n

Select thermodynamic components from the set:

Na2O MgO Al2O3 SiO2 K2O CaO TiO2 MnO FeO NiO ZrO2 Cl2
O2 H2O CuO Cr2O3 S2 F2 N2 ZnO

Enter names, 1 per line, press <enter> to finish:

MgO

CaO

Because the thermodynamic data file identifies: CO2 as special components, you will be prompted next for the EoS to be used for the corresponding components and mixtures thereof. To override this behavior, e.g., to use a generic hybrid fluid EoS, delete the special_component section from the thermodynamic data file header.

NOTE: the EoS choice specified here will override the EoS choice specified by the hybrid_EoS option, to override this behavior delete the special_component section from the the thermodynamic data file header.

Select fluid equation of state:

- 0 - X(CO2) H2O-CO2 Modified Redlich-Kwong (MRK) DeSantis et al 74
- 1 - X(CO2) H2O-CO2 HSMRK Kerrick & Jacobs 81
- 2 - X(CO2) H2O-CO2 MRK hybrid-EoS*
- 5 - X(CO2) H2O-CO2 CORK Holland & Powell 91, 98
- 8 - f(O2/CO2) C-buffered COH MRK hybrid-EoS*
- 10 - X(O) C-buffered COH MRK hybrid-EoS Connolly & Cesare 93*
- 12 - X(O)-f(S2) C-buffered COHS MRK hybrid-EoS Connolly & Cesare 93*
- 13 - X(H2) H2O-H2 MRK hybrid-EoS*
- 14 - X(CO2) H2O-CO2 Pitzer & Sterner 94; Holland & Powell mixing 03
- 15 - X(H2) H2O-H2 low T MRK hybrid-EoS*
- 16 - X(O) H-O MRK hybrid-EoS*
- 17 - X(O)-f(S2) H-O-S MRK hybrid-EoS*

- 19 - X(O)-X(S) C-buffered COHS MRK hybrid-EoS Connolly & Cesare 93*
- 20 - X(O)-X(C) COHS MRK hybrid-EoS Connolly & Cesare 93*
- 24 - f(O2/CO2)-N/C C-buffered COHN MRK hybrid-EoS*
- 25 - X(CO2)-X(NaCl) H2O-CO2-NaCl Aranovich et al 10
- 26 - X(O) O-Si MRK Connolly 16
- 27 - X(O)-X(C) C-O-H MRK hybrid-EoS*

*Hybrid EoS use the following pure species EoS, to change these associations modify the hybrid_EoS keywords in the perplex_option file:

- H2O - PSEoS Pitzer & Sterner 1994
- CO2 - PSEoS Pitzer & Sterner 1994
- CH4 - MRK DeSantis et al 1974

5

The data base has P(bar) and T(K) as default independent potentials.
Make one dependent on the other, e.g., as along a geothermal gradient (y/n)?

n

Specify number of independent potential variables:

- 0 - Composition diagram [default]
- 1 - Mixed-variable diagram
- 2 - Sections and Schreinemakers-type diagrams

2

Select x-axis variable:

- 1 - P(bar)
- 2 - T(K)
- 3 - Y(CO2)

*Although only one component is specified for the Y(CO2) phase, its equation of state permits use of its compositional variable:

2

Enter minimum and maximum values, respectively, for: T(K)

573

1273

Same T range as in Ex. 6

Select y-axis variable:

- 2 - P(bar)
- 3 - Y(CO2)

2

Enter minimum and maximum values, respectively, for: P(bar)

5000

30000

Same P range as in Ex. 6

Specify sectioning value for: Y(CO2)

1

Output a print file (Y/N)?

y

Exclude pure and/or endmember phases (Y/N)?

y

Do you want to be prompted for phases (Y/N)?

n

Enter names, 1 per line, press <enter> to finish:

per

dol

Same as in Ex. 6

Include solution models (Y/N)?

y

Enter the solution model file name [default = solution_model.dat]:

[enter]

...

Select models from the following list, enter 1 per line, press <enter> to finish

carbonate models: Do(AE) Cc(AE) oCcM(HP) Carb(M) oCcM(EF) dis(EF)

fluid models: COH-Fluid COH-Fluid+

For details on these models see: www.perplex.ethz.ch/perplex_solution_model_glossary.html
or read the commentary in the solution model file.

Do(AE)

Cc(AE)

Same as in Ex. 6

Enter calculation title:

ex7

(2) Doing the calculation (CONVEX)

Run CONVEX to make the calculation:

```
C:\PERPLEX\Perplex691>convex
```

Perple_X version 6.9.1, source updated January 3, 2022.

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Enter the project name (the name assigned in BUILD) [default = my_project]:

ex7

Reading problem definition from file: ex7.dat

Reading thermodynamic data from file: hp62ver.dat

Writing print output to file: ex7.plt

Writing plot output to file: ex7.plt

Reading solution models from file: solution_model.dat

Reading Perple_X options from: perplex_option.dat

Writing complete reaction list to: not requested
Writing auto refine summary to: ex7_auto_refine.txt
Writing pseudocompound glossary to: ex7_pseudocompound_glossary.txt
Writing Perple_X option summary to: not requested

Perple_X computational option settings for CONVEX:

Keyword: Value: Permitted values [default]:

Auto-refine options:

auto_refine aut [auto] manual off
replicate_threshold 0.1E-1 [1e-2]; static opt; <0 => no replica test
rep_dynamic_threshold 0.1E-2 [1d-3]; dynamic opt; <0 => no replica test
re-refine F [F] T
intermediate_savrpc F [F] T
intermediate_savdyn F [F] T
keep_all_rpcs T [T] F

Schreinemakers and Mixed-variable diagram options:

variance 1/99 [1/99], >0; maximum true variance
increment 0.100/0.025 [0.1/0.025], default search/trace variable increment
efficiency 3 [3] >0, <6
reaction_format min [min] full stoichiometry S+V everything
reaction_list off [off] on
console_messages on [on] off
short_print_file on [on] off

Solution subdivision options:

initial_resolution:
exploratory stage 0.0625 0->1 [1/16], 0 => off
auto-refine stage 0.0208 0->1 [], 0 => off
stretch_factor 0.0020 >0 [2d-3]
non_linear_switch F [F] T
subdivision_override off [off] lin str
hard_limits off [off] on
refine_endmembers F [F] T
pc_perturbation 0.0050 [5d-3]

Thermodynamic options:

solvus_tolerance aut [aut] or 0->1; aut = automatic, 0 => p=c pseudocompounds, 1 => homoge
T_stop (K) 0.0 [0]
T_melt (K) 873.0 [873]
approx_alpha T [T] F
Anderson-Gruneisen F [F] T
speciation_precision 0.1E-4 [1d-5] <1; absolute
speciation_max_it 100 [100]
GFSM F [F] T GFSM/special_component toggle
hybrid_EoS_H2O 4 [4] 0-2, 4-7
hybrid_EoS_CO2 4 [4] 0-4, 7
hybrid_EoS_CH4 0 [0] 0-1, 7
aq_bad_results err [err] 101 102 103 ignore
aq_lagged_speciation F [F] T
aq_ion_H+ T [T] F => use OH-
aq_oxide_components F [F] T
aq_solvent_solvus T [T] F
aq_vapor_epsilon 1.0 [1.]

Input/Output options:

pause_on_error T [T] F
timing T [T] F
auto_exclude T [T] F

To change these options see: www.perplex.ethz.ch/perplex_options.html

Solution model summary:

****warning ver114**** the following endmembers are missing for Do(AE)

sid

16 pseudocompounds generated for: Do(AE)

****warning ver114**** the following endmembers are missing for Cc(AE)

sid

16 pseudocompounds generated for: Cc(AE)

Total number of pseudocompounds: 32

Summary of included solution models:

Do(AE) Cc(AE)

**** Starting exploratory computational stage ****

cycle 1 1 1
cycle 2 2 2
cycle 3 3 3

Initial number of divariant assemblages to be tested is: 3

Testing divariant assemblage 1, 2 assemblages remaining to be tested.

Testing divariant assemblage 2, 2 assemblages remaining to be tested.

Testing divariant assemblage 3, 3 assemblages remaining to be tested.

Testing divariant assemblage 4, 4 assemblages remaining to be tested.

Testing divariant assemblage 5, 5 assemblages remaining to be tested.

Testing divariant assemblage 6, 6 assemblages remaining to be tested.

Testing divariant assemblage 7, 6 assemblages remaining to be tested.

****warning ver066**** Metastable assemblage into FLIPIT:

mag_6.2 cc

v = 7517.30 573.000 1.00000 0.00000 0.00000

Testing divariant assemblage 8, 6 assemblages remaining to be tested.

Testing divariant assemblage 9, 7 assemblages remaining to be tested.

****warning ver066**** Metastable assemblage into FLIPIT:

ma_98.50 arag

v = 30000.0 573.000 1.00000 0.00000 0.00000

Testing divariant assemblage 10, 8 assemblages remaining to be tested.

Testing divariant assemblage 11, 7 assemblages remaining to be tested.

Testing divariant assemblage 12, 7 assemblages remaining to be tested.

Testing divariant assemblage 13, 7 assemblages remaining to be tested.

Testing divariant assemblage 14, 6 assemblages remaining to be tested.

****warning ver066**** Metastable assemblage into FLIPIT:

mag_6.2 arag

v = 27500.0 1273.00 1.00000 0.00000 0.00000

Testing divariant assemblage 15, 5 assemblages remaining to be tested.

Testing divariant assemblage 16, 4 assemblages remaining to be tested.

Testing divariant assemblage 17, 5 assemblages remaining to be tested.

Testing divariant assemblage 18, 5 assemblages remaining to be tested.

Testing divariant assemblage 19, 4 assemblages remaining to be tested.

****warning ver066**** Metastable assemblage into FLIPIT:

mag_86.2 cc_55.1

v = 5000.00 1203.00 1.00000 0.00000 0.00000

Testing divariant assemblage 20, 3 assemblages remaining to be tested.

Testing divariant assemblage 21, 3 assemblages remaining to be tested.

Testing divariant assemblage 22, 3 assemblages remaining to be tested.

Testing divariant assemblage 23, 4 assemblages remaining to be tested.

Testing divariant assemblage 24, 3 assemblages remaining to be tested.

Testing divariant assemblage 25, 2 assemblages remaining to be tested.

Testing divariant assemblage 26, 2 assemblages remaining to be tested.

Testing divariant assemblage 27, 2 assemblages remaining to be tested.

Testing divariant assemblage 28, 1 assemblages remaining to be tested.

****warning ver066**** Metastable assemblage into FLIPIT:

arag mag_18.5

v = 30000.0 1133.00 1.00000 0.00000 0.00000

Testing divariant assemblage 29, 0 assemblages remaining to be tested.

Compositions for simplicial model: Do(AE)

	Minimum	Maximum
--	---------	---------

cc	0.49000	0.55125
----	---------	---------

mag	0.44875	0.51000
-----	---------	---------

Compositions for simplicial model: Cc(AE)

	Minimum	Maximum
--	---------	---------

mag	0.61562E-01	0.98500
-----	-------------	---------

cc	0.15000E-01	0.93844
----	-------------	---------

Solution model summary:

10 pseudocompounds generated for: Do(AE)

48 pseudocompounds generated for: Cc(AE)

Total number of pseudocompounds: 58

Summary of included solution models:

Do(AE) Cc(AE)

**** Starting auto_refine computational stage ****

cycle	1	1	1
-------	---	---	---

cycle	2	2	2
-------	---	---	---

cycle	3	3	3
-------	---	---	---

cycle	4	4	4
-------	---	---	---

Initial number of divariant assemblages to be tested is: 4

Testing divariant assemblage 1, 3 assemblages remaining to be tested.

finished with equilibrium (1) Cc(AE)(mag) arag = Cc(AE)(ma_98.50)

Testing divariant assemblage 2, 3 assemblages remaining to be tested.

finished with equilibrium (2) Cc(AE)(ma_98.50) Do(AE)(cc_49.0) = Cc(AE)(mag_96.4)

finished with equilibrium (3) Cc(AE)(ma_98.50) arag = Do(AE)(cc_49.0)

finished with equilibrium (4) Cc(AE)(ma_98.50) arag = Cc(AE)(mag_96.4)

finished with equilibrium (5) Cc(AE)(mag_96.4) arag = Do(AE)(cc_49.0)

Testing divariant assemblage 3, 4 assemblages remaining to be tested.

finished with equilibrium (6) Do(AE)(cc_49.0) Cc(AE)(mag_2.1) = Do(AE)(cc_51.0)

finished with equilibrium (7) Do(AE)(cc_49.0) arag = Cc(AE)(mag_2.1)

finished with equilibrium (8) Do(AE)(cc_49.0) arag = Do(AE)(cc_51.0)

finished with equilibrium (9) Do(AE)(cc_51.0) arag = Cc(AE)(mag_2.1)

finished with equilibrium (10) Cc(AE)(mag_2.1) Do(AE)(cc_51.0) = Cc(AE)(mag_4.1)

finished with equilibrium (11) arag Cc(AE)(mag_4.1) = Cc(AE)(mag_2.1)

finished with equilibrium (12) Do(AE)(cc_51.0) arag = Cc(AE)(mag_4.1)

finished with equilibrium (13) Do(AE)(cc_51.0) arag = Cc(AE)(mag_6.2)

finished with equilibrium (14) Do(AE)(cc_51.0) Cc(AE)(mag_4.1) = Cc(AE)(mag_6.2)

finished with equilibrium (15) arag Cc(AE)(mag_6.2) = Cc(AE)(mag_4.1)

finished with equilibrium (16) Do(AE)(cc_51.0) arag = Do(AE)(cc_53.1)

finished with equilibrium (17) Do(AE)(cc_51.0) Cc(AE)(mag_6.2) = Do(AE)(cc_53.1)

finished with equilibrium (18) arag Do(AE)(cc_53.1) = Cc(AE)(mag_6.2)

finished with equilibrium (19) arag Cc(AE)(mag_8.2) = Cc(AE)(mag_6.2)

finished with equilibrium (20) arag Do(AE)(cc_53.1) = Cc(AE)(mag_8.2)

finished with equilibrium (21) Cc(AE)(mag_6.2) Do(AE)(cc_53.1) = Cc(AE)(mag_8.2)

finished with equilibrium (22) arag Do(AE)(cc_53.1) = Cc(AE)(mag_10.3)

finished with equilibrium (23) arag Cc(AE)(mag_10.3) = Cc(AE)(mag_8.2)

finished with equilibrium (24) Do(AE)(cc_53.1) Cc(AE)(mag_8.2) = Cc(AE)(mag_10.3)

finished with equilibrium (25) arag Do(AE)(cc_53.1) = Do(AE)(cc_55.1)

finished with equilibrium (26) arag Do(AE)(cc_55.1) = Cc(AE)(mag_10.3)

finished with equilibrium (27) Do(AE)(cc_53.1) Cc(AE)(mag_10.3) = Do(AE)(cc_55.1)

finished with equilibrium (28) arag Cc(AE)(mag_12.3) = Cc(AE)(mag_10.3)

finished with equilibrium (29) arag Do(AE)(cc_55.1) = Cc(AE)(mag_12.3)

finished with equilibrium (30) Cc(AE)(mag_10.3) Do(AE)(cc_55.1) = Cc(AE)(mag_12.3)

finished with equilibrium (31) arag Do(AE)(cc_55.1) = Cc(AE)(mag_14.4)

finished with equilibrium (32) arag Cc(AE)(mag_14.4) = Cc(AE)(mag_12.3)

finished with equilibrium (33) Do(AE)(cc_55.1) Cc(AE)(mag_12.3) = Cc(AE)(mag_14.4)

finished with equilibrium (34) arag Do(AE)(cc_55.1) = Cc(AE)(mag_16.4)

finished with equilibrium (35) arag Cc(AE)(mag_16.4) = Cc(AE)(mag_14.4)

finished with equilibrium (36) Do(AE)(cc_55.1) Cc(AE)(mag_14.4) = Cc(AE)(mag_16.4)

Testing divariant assemblage 4, 5 assemblages remaining to be tested.

finished with equilibrium (37) arag = Cc(AE)(cc)

Testing divariant assemblage 5, 5 assemblages remaining to be tested.

Testing divariant assemblage 6, 6 assemblages remaining to be tested.

finished with equilibrium (38) Do(AE)(cc_49.0) = Cc(AE)(mag_96.4) Do(AE)(cc_51.0)

Testing divariant assemblage 7, 7 assemblages remaining to be tested.

Testing divariant assemblage 8, 6 assemblages remaining to be tested.

Testing divariant assemblage 9, 7 assemblages remaining to be tested.

Testing divariant assemblage 10, 6 assemblages remaining to be tested.

Testing divariant assemblage 11, 6 assemblages remaining to be tested.

Testing divariant assemblage 12, 7 assemblages remaining to be tested.

Testing divariant assemblage 13, 6 assemblages remaining to be tested.

finished with equilibrium (39) Cc(AE)(mag_96.4) Do(AE)(cc_51.0) = Cc(AE)(mag_94.4)

Testing divariant assemblage 14, 9 assemblages remaining to be tested.

Testing divariant assemblage 15, 8 assemblages remaining to be tested.

Testing divariant assemblage 16, 7 assemblages remaining to be tested.

Testing divariant assemblage 17, 8 assemblages remaining to be tested.

Testing divariant assemblage 18, 8 assemblages remaining to be tested.

Testing divariant assemblage 19, 9 assemblages remaining to be tested.

Testing divariant assemblage 20, 8 assemblages remaining to be tested.

finished with equilibrium (40) Cc(AE)(mag_94.4) Do(AE)(cc_51.0) = Cc(AE)(mag_92.3)

Testing divariant assemblage 21, 10 assemblages remaining to be tested.

Testing divariant assemblage 22, 9 assemblages remaining to be tested.

Testing divariant assemblage 23, 8 assemblages remaining to be tested.
Testing divariant assemblage 24, 7 assemblages remaining to be tested.
Testing divariant assemblage 25, 8 assemblages remaining to be tested.
Testing divariant assemblage 26, 7 assemblages remaining to be tested.
Testing divariant assemblage 27, 7 assemblages remaining to be tested.
Testing divariant assemblage 28, 7 assemblages remaining to be tested.
Testing divariant assemblage 29, 6 assemblages remaining to be tested.
finished with equilibrium (41) $Cc(AE)(mag_92.3) Do(AE)(cc_51.0) = Cc(AE)(mag_90.3)$
Testing divariant assemblage 30, 8 assemblages remaining to be tested.
Testing divariant assemblage 31, 7 assemblages remaining to be tested.
Testing divariant assemblage 32, 7 assemblages remaining to be tested.
Testing divariant assemblage 33, 7 assemblages remaining to be tested.
Testing divariant assemblage 34, 8 assemblages remaining to be tested.
Testing divariant assemblage 35, 8 assemblages remaining to be tested.
Testing divariant assemblage 36, 7 assemblages remaining to be tested.
finished with equilibrium (42) $Cc(AE)(mag_90.3) Do(AE)(cc_51.0) = Cc(AE)(mag_88.2)$
Testing divariant assemblage 37, 9 assemblages remaining to be tested.
Testing divariant assemblage 38, 8 assemblages remaining to be tested.
Testing divariant assemblage 39, 8 assemblages remaining to be tested.
Testing divariant assemblage 40, 7 assemblages remaining to be tested.
Testing divariant assemblage 41, 6 assemblages remaining to be tested.
Testing divariant assemblage 42, 5 assemblages remaining to be tested.
Testing divariant assemblage 43, 6 assemblages remaining to be tested.
Testing divariant assemblage 44, 6 assemblages remaining to be tested.
finished with equilibrium (43) $Cc(AE)(mag_88.2) Do(AE)(cc_51.0) = Cc(AE)(mag_86.2)$
Testing divariant assemblage 45, 8 assemblages remaining to be tested.
Testing divariant assemblage 46, 7 assemblages remaining to be tested.
Testing divariant assemblage 47, 6 assemblages remaining to be tested.
Testing divariant assemblage 48, 6 assemblages remaining to be tested.
Testing divariant assemblage 49, 7 assemblages remaining to be tested.
Testing divariant assemblage 50, 7 assemblages remaining to be tested.
Testing divariant assemblage 51, 7 assemblages remaining to be tested.
warning ver066 Metastable assemblage into FLIPIT:
mag_86.2 cc_51.0
v = 5000.00 1255.50 1.00000 0.00000 0.00000
Testing divariant assemblage 52, 6 assemblages remaining to be tested.
warning ver066 Metastable assemblage into FLIPIT:
mag_86.2 mag_88.2
v = 5000.00 1255.50 1.00000 0.00000 0.00000
Testing divariant assemblage 53, 5 assemblages remaining to be tested.
Testing divariant assemblage 54, 5 assemblages remaining to be tested.
Testing divariant assemblage 55, 4 assemblages remaining to be tested.
Testing divariant assemblage 56, 4 assemblages remaining to be tested.
Testing divariant assemblage 57, 5 assemblages remaining to be tested.
Testing divariant assemblage 58, 4 assemblages remaining to be tested.
Testing divariant assemblage 59, 4 assemblages remaining to be tested.
Testing divariant assemblage 60, 4 assemblages remaining to be tested.
Testing divariant assemblage 61, 3 assemblages remaining to be tested.
Testing divariant assemblage 62, 3 assemblages remaining to be tested.
Testing divariant assemblage 63, 4 assemblages remaining to be tested.
Testing divariant assemblage 64, 4 assemblages remaining to be tested.

Testing divariant assemblage 65, 3 assemblages remaining to be tested.
 Testing divariant assemblage 66, 2 assemblages remaining to be tested.
 Testing divariant assemblage 67, 3 assemblages remaining to be tested.
 Testing divariant assemblage 68, 3 assemblages remaining to be tested.
 Testing divariant assemblage 69, 2 assemblages remaining to be tested.
 finished with equilibrium (44) Cc(AE)(mag_16.4) Do(AE)(cc_55.1) = Cc(AE)(mag_18.5)
 Testing divariant assemblage 70, 4 assemblages remaining to be tested.
 Testing divariant assemblage 71, 4 assemblages remaining to be tested.
 Testing divariant assemblage 72, 3 assemblages remaining to be tested.
 finished with equilibrium (45) Cc(AE)(mag_18.5) Do(AE)(cc_55.1) = Do(AE)(cc_57.2)
 Testing divariant assemblage 73, 5 assemblages remaining to be tested.
 Testing divariant assemblage 74, 4 assemblages remaining to be tested.
 Testing divariant assemblage 75, 4 assemblages remaining to be tested.
 ***warning ver066** Metastable assemblage into FLIPIT:
 mag_16.4 arag
 v = 30000.0 1150.50 1.00000 0.00000 0.00000
 Testing divariant assemblage 76, 3 assemblages remaining to be tested.
 Testing divariant assemblage 77, 2 assemblages remaining to be tested.
 finished with equilibrium (46) Do(AE)(cc_57.2) Cc(AE)(mag_18.5) = Cc(AE)(mag_20.5)
 Testing divariant assemblage 78, 4 assemblages remaining to be tested.
 Testing divariant assemblage 79, 4 assemblages remaining to be tested.
 Testing divariant assemblage 80, 4 assemblages remaining to be tested.
 Testing divariant assemblage 81, 3 assemblages remaining to be tested.
 Testing divariant assemblage 82, 3 assemblages remaining to be tested.
 Testing divariant assemblage 83, 3 assemblages remaining to be tested.
 Testing divariant assemblage 84, 3 assemblages remaining to be tested.
 Testing divariant assemblage 85, 2 assemblages remaining to be tested.
 Testing divariant assemblage 86, 2 assemblages remaining to be tested.
 Testing divariant assemblage 87, 2 assemblages remaining to be tested.
 Testing divariant assemblage 88, 2 assemblages remaining to be tested.
 Testing divariant assemblage 89, 2 assemblages remaining to be tested.
 Testing divariant assemblage 90, 1 assemblages remaining to be tested.
 Testing divariant assemblage 91, 0 assemblages remaining to be tested.

Compositions for simplicial model: Do(AE)

	Minimum	Maximum
cc	0.49000	0.57167
mag	0.42833	0.51000

Compositions for simplicial model: Cc(AE)

	Minimum	Maximum
mag	0.20521E-01	0.98500
cc	0.15000E-01	0.97948

(3) Plotting the calculated phase diagram (PSVDRAW)

Run PSVDRAW to plot the calculated pseudosection:

C:\PERPLEX\Perplex691>psvdraw

Perple_X version 6.9.1, source updated January 3, 2022.

Enter the project or plot file name [i.e., without the .plt suffix]:

ex7

Perple_X plot options are currently set as:

Keyword:	Value:	Permitted values [default]:
axis_label_scale	1.20	[1.2] (rel)
bounding_box :		
	0	[0] x-min (pts)
	0	[0] y-min (pts)
	800	[800] x-length (pts)
	800	[800] y-length (pts)
field_fill	T	[T] F
field_label	T	[T] F
numeric_field_label	F	[F] T, if T PSSECT writes list to *_assemblages.txt
replicate_label	0.250	0->1 [0.025]
field_label_scale	0.75	[0.72] (rel)
font	Helvetica	
grid	F	[F] T
half_ticks	T	[T] F
line_width	1.00	0-99 [1.] (pts)
picture_transformation :		
	0.180	[0.18] x-scale (rel)
	0.180	[0.18] y-scale (rel)
	130.	[0.18] x-translation (pts)
	220.	[0.18] y-translation (pts)
	0.00	[0.0] rotation (deg)
plot_aspect_ratio	1.000	[1.0] x_axis_length/y_axis_length
splines	T	[T] F
tenth_ticks	F	[F] T
text_scale	1.000	[1.] (rel)
plot_extra_data		

To change these options edit or create the plot option file

See: www.perplex.ethz.ch/perplex_plot_options.html

PostScript will be written to file: ex7.ps

Modify the default plot (y/n)?

Y

CONVEX has calculated both true univariant equilibria (i.e. variance = 1) and **pseudo-univariant equilibria (i.e. equilibria among pseudocompounds, involving two pseudocompounds of the same phase on both sides of the reaction; variance =2)**. Pseudo-univariant equilibria are not true univariant reactions, and it is convenient not to plot them, otherwise the resulting diagram would be full of curves.

Modify drafting options (y/n)?

answer yes to modify:

- field labeling
- x-y plotting limits
- axes numbering

n

Restrict phase fields by variance (y/n)?

answer yes to:

- suppress pseudounivariant curves and/or pseudoinvariant points of a specified true variance.

y

This is a key prompt. We are interested to “true” univariant reactions (i.e. true variance = 1), not to pseudo-univariant curves (i.e. di-variant equilibria involving two pseudocompounds of the same phase on both sides of the reaction). Therefore we must suppress all the curves that have a variance ≥ 2 (i.e. we must show all fields with true variance < 2 , see below).

Select true variance restriction to be applied to pseudo-invariant/univariant equilibria:

- 1 - show all fields with true variance $<$ than a specified value [default]
- 2 - show all fields with a specified true variance

1

We are interested to “true” univariant reactions (i.e. true variance = 1), therefore we must show all fields with true variance < 2 .

Enter the true variance to be used for this restriction [1-99, default = 2]:

2

Suppress pseudoinvariant points (y/n)?

N

Pseudoinvariant points are useful for visualizing how a phase changes its composition along a true univariant curve (see below).

Restrict phase fields by phase identities (y/n)?

answer yes to:

- show fields that contain a specific assemblage
- show fields that do not contain specified phases
- show fields that contain any of a set of specified phases

n

Modify default equilibrium labeling (y/n)?

answer yes to:

- modify/suppress [pseudo-] univariant curve labels
- suppress [pseudo-] invariant point labels

y

Suppress curve labels (y/n)?

n

Change default labeling of curve segments (y/n)?

y

Suppress labels of pseudounivariant curves (y/n)?

y

Enter minimum fraction of the axes length that a

curve must be to receive a text label (0-1):

1 means that a text label will be assigned to those curves that are longer than the axes length.

1

Enter minimum fraction of the axes length that a curve must be to receive a numeric label (0-1.000):

0 means that a numeric label will be assigned to all those curves that are shorter than the axes length.

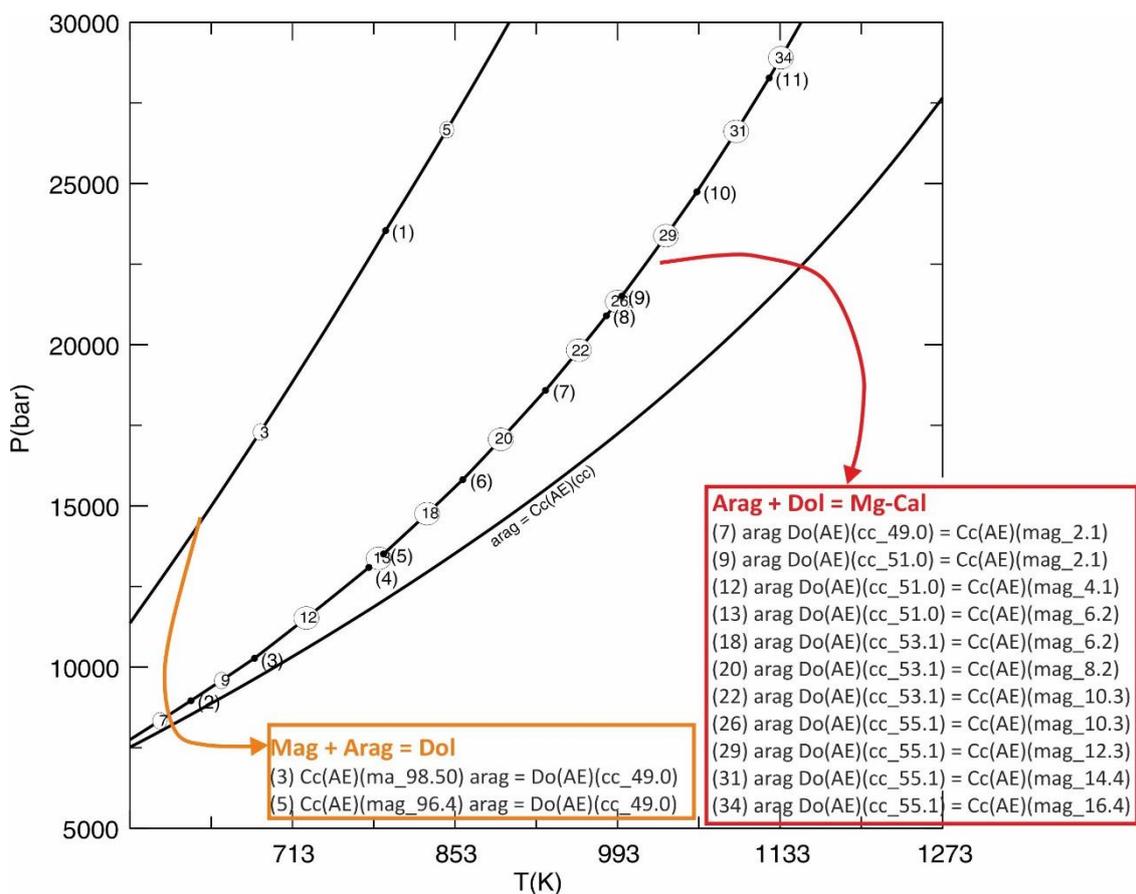
0

Suppress point labels (y/n)?

N

The resulting diagram shows three univariant equilibria. Two of them are divided in several parts (each one with a numeric label) by pseudo-invariant points (small points, with number in brackets). The third univariant equilibrium is the polymorphic transformation of calcite to aragonite.

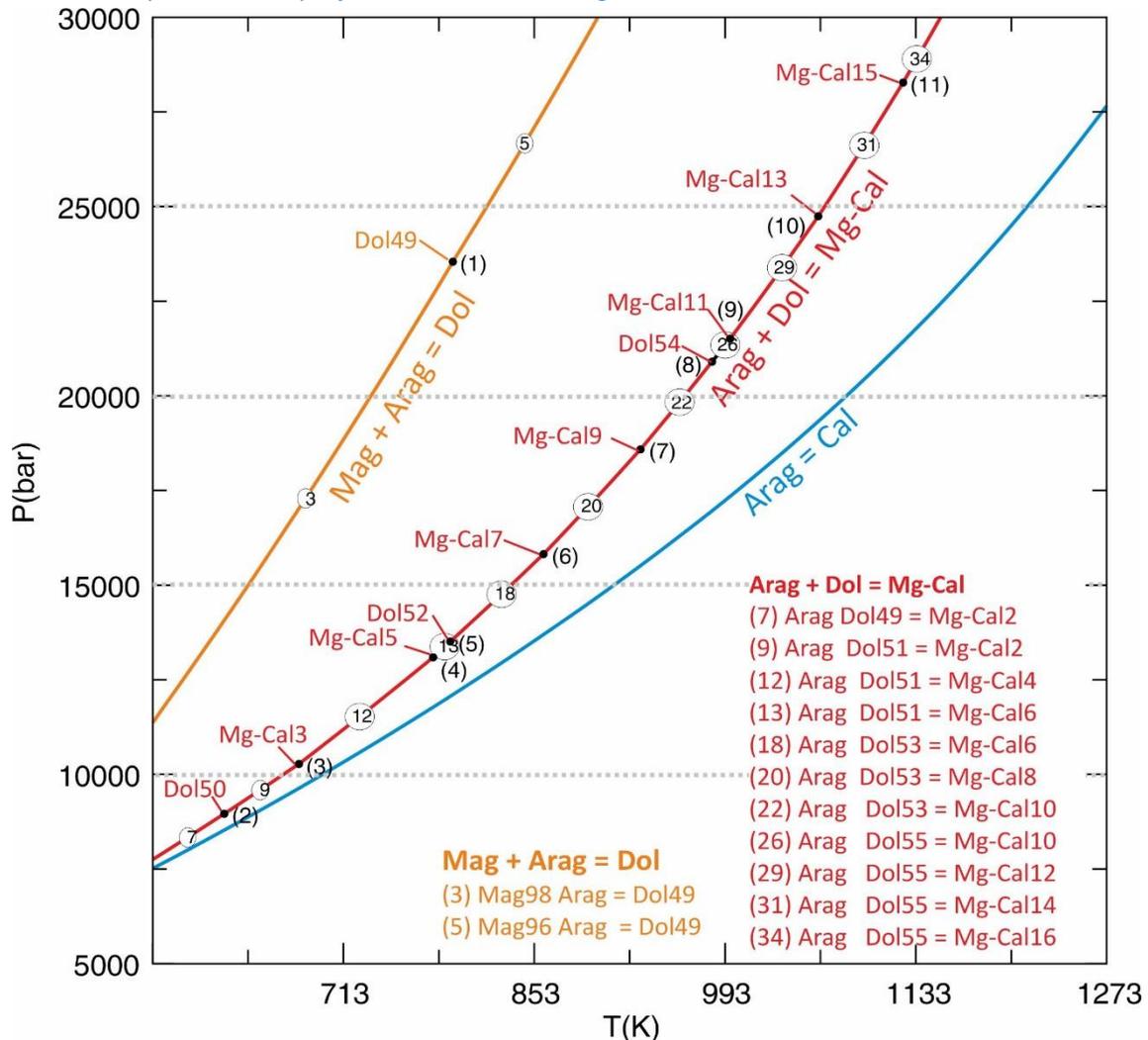
To understand the meaning of each part of the univariant equilibria, open the ex7.prn file. At the end of this file, the (pseudo-) univariant equilibria are summarized.



Note that each segment of the same univariant curve differs from the others for the composition of one phase. This implies that the composition of solid solutions (Mg-calcite, dolomite and magnesite) changes along each univariant curve (as in all P-T projections involving solid solutions!).

(4) Comparing T-X sections and P-T projections

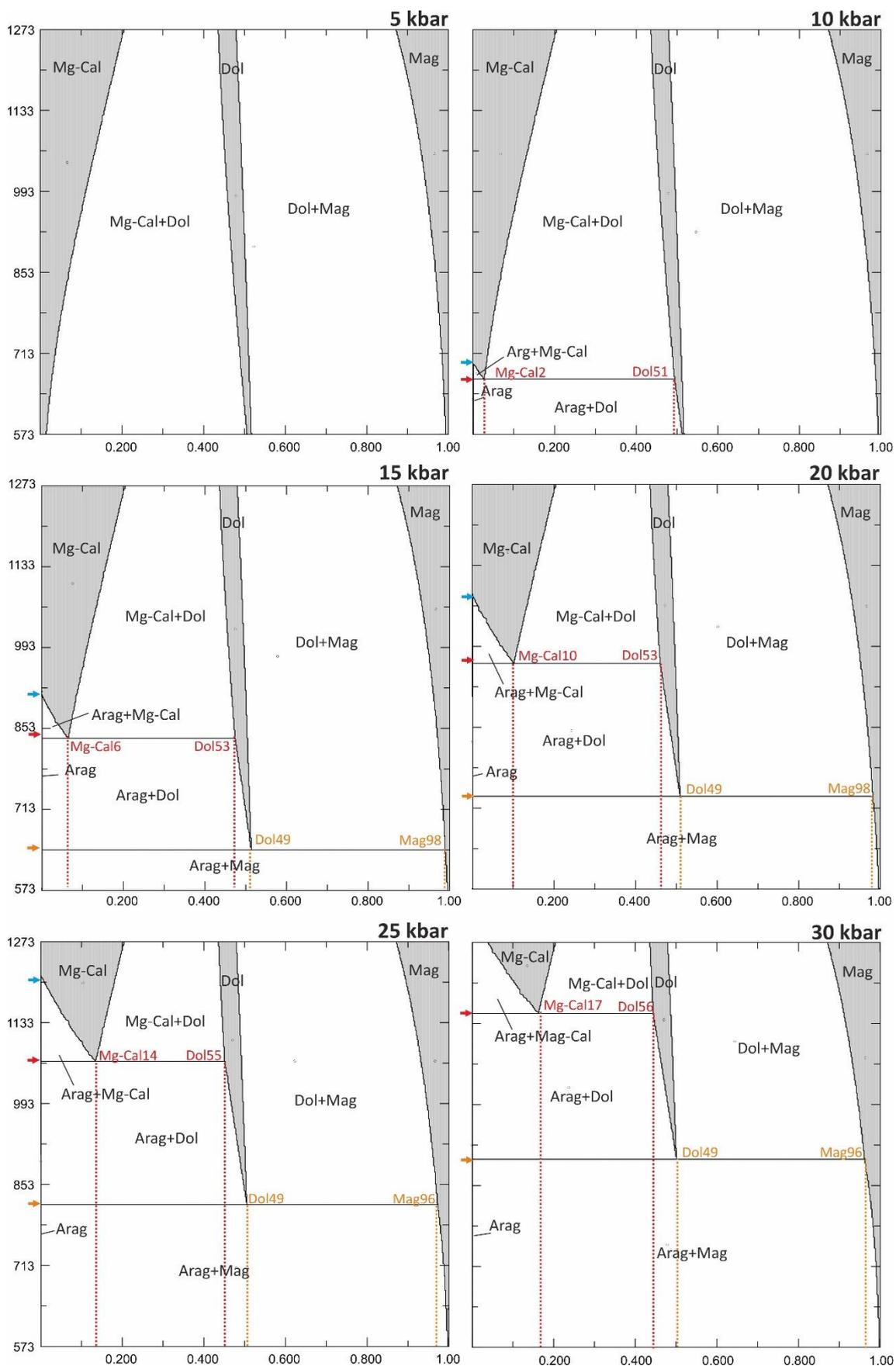
You can now compare the P-T projection with the T-XMgO sections obtained in Ex. 6.



Note that the two types of diagram provide the same information, but in different way.

In the **P-T projection**, the solid solutions compositional information is somehow “hidden”: you can understand how solid solutions change their composition as a function of P and T by carefully analysing each segment of the univariant curves.

In the **isobaric T-X sections**, solid solutions compositions are explicitly indicated, but you need more than one diagram to understand how these compositions change as a function of pressure.



Ex 8

Ex. 8 – AFM chemographies in the KFMASH system

This exercise explains how to calculate the “classical” Thompson AFM diagrams for metapelites in the KFMASH system. Opposite to Ex. 3, solid solutions are considered.

COMPONENT TRANSFORMATIONS are necessary in order to compute these phase diagrams. In the classical AFM projection, compositions are reduced through the projection hierarchy H₂O, SiO₂ (q), KAl₃O₅ (mu) into the sub-composition MgO-FeO-Al₂O₃.

(1) Projection through muscovite implies that a **muscovite component must be defined (MU = 0.5 K₂O + 1.5 Al₂O₃)**. Along the KAl₃O₅-SiO₂ join, K-feldspar has a negative composition and it will be therefore rejected. This means that **the calculation will only be valid within the stability field for Mu + Qz**.

(2) Projecting from muscovite into the AFM space, biotite has a negative composition and would be excluded by CONVEX. This problem is circumvented by defining two components, **PHL (= 1.5 MgO – 0.5Al₂O₃)** and **ANN (= 1.5 FeO – 0.5Al₂O₃)**, to replace the normal FeO and MgO components, so that biotite plots inside the composition space considered by CONVEX.

(1) Definition of the problem (BUILD)

```
C:\PERPLEX\Perplex691>build
```

Perple_X version 6.9.1, source updated January 3, 2022.

Copyright (C) 1986-2022 James A D Connolly <www.perplex.ethz.ch/copyright.html>.

NO is the default (blank) answer to all Y/N prompts

Enter a name for this project (the name will be used as the root for all output file names) [default = my_project]:

```
ex8
```

The problem definition file will be named: ex8.dat

Enter thermodynamic data file name [default = hp02ver.dat]:

```
hp62ver.dat
```

Enter the computational option file name [default = perplex_option.dat]:

See: www.perplex.ethz.ch/perplex_options.html

Reading Perple_X options from: perplex_option.dat

The current data base components are:

Na₂O MgO Al₂O₃ SiO₂ K₂O CaO TiO₂ MnO FeO NiO ZrO₂ Cl₂ O₂ H₂O CO₂ CuO Cr₂O₃ S₂ F₂ N₂ ZnO

Transform them (Y/N)?

Y

Three new components should be defined here:



MU will be defined by replacing the normal K₂O component, whereas PHL and ANN are defined by replacing the normal MgO and FeO components.

Enter new component name, < 6 characters, left justified:

MU

Enter old component to be replaced with MU :

K₂O

Enter other components (< 13) in MU 1 per line, <enter> to finish:

Al₂O₃

Enter stoichiometric coefficients of:

K₂O Al₂O₃

in MU (in above order):

Muscovite has the formula: $\text{KAl}_3\text{Si}_3\text{O}_{10}(\text{OH})_2$; if SiO₂ and H₂O are considered in excess, its composition is defined by $0.5 \text{ K}_2\text{O} + 1.5 \text{ Al}_2\text{O}_3$ (KAl₃O₅)

0.5

1.5



Is this correct (Y/N)?

Y

The current data base components are:

Na₂O MgO Al₂O₃ SiO₂ MU CaO TiO₂ MnO FeO NiO ZrO₂ Cl₂ O₂ H₂O CO₂ CuO Cr₂O₃ S₂ F₂ N₂ ZnO

Transform them (Y/N)?

Note that the newly defined MU component has replaced K₂O in the list of the database components.

Y

Enter new component name, < 6 characters, left justified:

PHL

Enter old component to be replaced with PHL :

MgO

Enter other components (< 13) in PHL 1 per line, <enter> to finish:

Al₂O₃

Enter stoichiometric coefficients of:

MgO Al₂O₃

in PHL (in above order):

Phlogopite has the formula: $\text{KMg}_3\text{AlSi}_3\text{O}_{10}(\text{OH})_2$. Considering H₂O, SiO₂ and KAl₃O₅ in excess, its composition is defined as $\text{PHL} = (3\text{MgO} - \text{Al}_2\text{O}_3)$ or, reduced, $\text{PHL} = (1.5\text{MgO} - 0.5\text{Al}_2\text{O}_3)$.

1.5

-0.5

PHL = 1.50 MgO -0.50 Al2O3

Is this correct (Y/N)?

y

The current data base components are:

Na2O PHL Al2O3 SiO2 MU CaO TiO2 MnO FeO NiO ZrO2 Cl2 O2 H2O CO2 CuO Cr2O3 S2 F2 N2 ZnO

Transform them (Y/N)?

Y

Enter new component name, < 6 characters, left justified:

ANN

Enter old component to be replaced with ANN :

FeO

Enter other components (< 13) in ANN 1 per line, <enter> to finish:

Al2O3

Enter stoichiometric coefficients of:

FeO Al2O3

in ANN (in above order):

Annite has the formula: $KFe_3AlSi_3O_{10}(OH)_2$. Considering H2O, SiO2 and KAl3O5 in excess, its composition is defined as ANN = (3FeO – Al2O3) or, reduced, ANN = (1.5FeO – 0.5Al2O3).

1.5

-0.5

ANN = 1.50 FeO -0.50 Al2O3

Is this correct (Y/N)?

y

The current data base components are:

Na2O PHL Al2O3 SiO2 MU CaO TiO2 MnO ANN NiO ZrO2 Cl2 O2 H2O CO2 CuO Cr2O3 S2 F2 N2 ZnO

Transform them (Y/N)?

Note that the newly defined ANN component has replaced FeO in the list of the database components.

n

Specify computational mode:

- 1 - Convex-Hull minimization
- 2 - Constrained minimization on a 2d grid [default]
- 3 - Constrained minimization on a 1d grid
- 4 - Output pseudocompound data
- 5 - 1-d Phase fractionation
- 6 - 0-d Infiltration-reaction-fractionation
- 7 - 2-d Phase fractionation (FRAC2D and TITRATE reactive transport models)

Use Convex-Hull minimization for Schreinemakers projections or phase diagrams with > 2 independent variables. Use constrained minimization for phase diagrams or phase diagram sections with < 3 independent variables.

1

Calculations with a saturated fluid (Y/N)?

y

Select the independent saturated fluid components:

H2O CO2

Enter names, 1 per line, press <enter> to finish:

For C-O-H fluids it is only necessary to select volatile species present in the solids of interest. If the species listed here are H2O and CO2, then to constrain O2 chemical potential to be consistent with C-O-H fluid speciation treat O2 as a saturated component. Refer to the Perple_X Tutorial for details.

H2O

Calculations with saturated components (Y/N)?

y

SiO2 and MU (KAl3O5) must be considered as saturated component, in this specific order.

****warning ver015**** if you select > 1 saturated component, then the order you enter the components determines the saturation hierarchy and may effect your results (see Connolly 1990).

Select < 6 saturated components from the set:

Na2O PHL Al2O3 CaO TiO2 MnO ANN NiO ZrO2 Cl2 O2 CO2 CuO Cr2O3 S2 F2 N2 ZnO

Enter names, 1 per line, press <enter> to finish:

SiO2

MU

Use chemical potentials, activities or fugacities as independent variables (Y/N)?

n

Select thermodynamic components from the set:

Na2O PHL Al2O3 CaO TiO2 MnO ANN NiO ZrO2 Cl2 O2 CO2 CuO Cr2O3 S2 F2 N2 ZnO

Enter names, 1 per line, press <enter> to finish:

ANN

PHL

Al2O3

The order (1st, 2nd, 3rd) influences how the three components are plotted in the chemographies: first = bottom left, second = bottom right, third = top.

Because the thermodynamic data file identifies: H2O as special components, you will be prompted next for the EoS to be used for the corresponding components and mixtures thereof. To override this behavior, e.g., to use a generic hybrid fluid EoS, delete the special_component section from the thermodynamic data file header.

NOTE: the EoS choice specified here will override the EoS choice specified by the hybrid_EoS option, to override this behavior delete the special_component section from the the thermodynamic data file header.

Select fluid equation of state:

0 - X(CO2) H2O-CO2 Modified Redlich-Kwong (MRK) DeSantis et al 74

1 - X(CO2) H2O-CO2 HSMRK Kerrick & Jacobs 81

2 - X(CO2) H2O-CO2 MRK hybrid-EoS*

5 - X(CO2) H2O-CO2 CORK Holland & Powell 91, 98

8 - f(O2/CO2) C-buffered COH MRK hybrid-EoS*

10 - X(O) C-buffered COH MRK hybrid-EoS Connolly & Cesare 93*

12 - X(O)-f(S2) C-buffered COHS MRK hybrid-EoS Connolly & Cesare 93*

13 - X(H2) H2O-H2 MRK hybrid-EoS*

- 14 - X(CO2) H2O-CO2 Pitzer & Sterner 94; Holland & Powell mixing 03
- 15 - X(H2) H2O-H2 low T MRK hybrid-EoS*
- 16 - X(O) H-O MRK hybrid-EoS*
- 17 - X(O)-f(S2) H-O-S MRK hybrid-EoS*
- 19 - X(O)-X(S) C-buffered COHS MRK hybrid-EoS Connolly & Cesare 93*
- 20 - X(O)-X(C) COHS MRK hybrid-EoS Connolly & Cesare 93*
- 24 - f(O2/CO2)-N/C C-buffered COHN MRK hybrid-EoS*
- 25 - X(CO2)-X(NaCl) H2O-CO2-NaCl Aranovich et al 10
- 26 - X(O) O-Si MRK Connolly 16
- 27 - X(O)-X(C) C-O-H MRK hybrid-EoS*

*Hybrid EoS use the following pure species EoS, to change these associations modify the hybrid_EoS keywords in the perplex_option file:

- H2O - PEoS Pitzer & Sterner 1994
- CO2 - PEoS Pitzer & Sterner 1994
- CH4 - MRK DeSantis et al 1974

5

The data base has P(bar) and T(K) as default independent potentials.
Make one dependent on the other, e.g., as along a geothermal gradient (y/n)?

n

Specify number of independent potential variables:

- 0 - Composition diagram [default]
- 1 - Mixed-variable diagram
- 2 - Sections and Schreinemakers-type diagrams

0

Output a print file (Y/N)?

y

Exclude pure and/or endmember phases (Y/N)?

y

Do you want to be prompted for phases (Y/N)?

n

Enter names, 1 per line, press <enter> to finish:

Exclude K-bearing phases other than muscovite and biotite.

- fstp | Fe-stilpnomelane
- mstp | Mg-stilpnomelane
- cel | celadonite KMgAlSi4O10(OH)2
- fcel | Fe-celadonite KFeAlSi4O10(OH)2
- kcm | K-cymrite KAlSi3O8 · H2O
- wa | wadeleite K2Si4O9
- hol | hollandite KAlSi3O8
- kls | kalsilite KAlSiO4
- lc | leucite KAlSi2O6
- kjdh | make-definition for Holland et al., 2018 Cpx solution model
- kjL | make-definition for Holland et al., 2018 melt solution model
- kspL | K-feldspar liquid

Include solution models (Y/N)?

y

Enter the solution model file name [default = solution_model.dat]:

[enter]

...

Select models from the following list, enter 1 per line, press <enter> to finish

clinoamphibole models: cAmph_I(G) cAmph(G) Cumm cAmph(DP) cAmph_I(DP)

clinopyroxene models: Cpx_I(HGP) Cpx(HGP) Augite(G) Cpx(JH)

...

...

For details on these models see: www.perplex.ethz.ch/perplex_solution_model_glossary.html or read the commentary in the solution model file.

Chl(W)

Bi(W)

Gt(W)

Ctd(W)

St(W)

Crd(W)

Enter calculation title:

Ex8

*Although only one component is specified for the fluid phase, its equation of state permits use of its compositional variable: Y(CO₂) .

Specify values for:

P(bar) T(K) Y(CO₂)

For calculation 1, enter zeros to finish.

8000

843

0

Specify values for:

P(bar) T(K) Y(CO₂)

For calculation 2, enter zeros to finish.

8000

853

0

Specify values for:

P(bar) T(K) Y(CO₂)

For calculation 3, enter zeros to finish.

8000

863

0

Specify values for:

P(bar) T(K) Y(CO2)

For calculation 4, enter zeros to finish.

8000

873

0

Specify values for:

P(bar) T(K) Y(CO2)

For calculation 6, enter zeros to finish.

0

0

0

(2) Doing the calculation (CONVEX)

Run CONVEX to make the calculation:

```
C:\PERPLEX\Perplex691>convex
```

Perple_X version 6.9.1, source updated January 3, 2022.

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Enter the project name (the name assigned in BUILD) [default = my_project]:

ex8

Reading problem definition from file: ex8.dat

Reading thermodynamic data from file: hp62ver.dat

Writing print output to file: ex8.plt

Writing plot output to file: ex8.plt

Reading solution models from file: solution_model.dat

Reading Perple_X options from: perplex_option.dat

Writing auto refine summary to: ex8_auto_refine.txt

Writing pseudocompound glossary to: ex8_pseudocompound_glossary.txt

Writing Perple_X option summary to: not requested

Perple_X computational option settings for CONVEX:

Keyword: Value: Permitted values [default]:

Auto-refine options:

auto_refine aut [auto] manual off

replicate_threshold 0.1E-1 [1e-2]; static opt; <0 => no replica test

rep_dynamic_threshold 0.1E-2 [1d-3]; dynamic opt; <0 => no replica test

re-refine F [F] T

intermediate_savrpc F [F] T

intermediate_savdyn F [F] T

keep_all_rpcs T [T] F

Solution subdivision options:

initial_resolution:

exploratory stage 0.0625 0->1 [1/16], 0 => off
auto-refine stage 0.0063 0->1 [], 0 => off
stretch_factor 0.0020 >0 [2d-3]
non_linear_switch F [F] T
subdivision_override off [off] lin str
hard_limits off [off] on
refine_endmembers F [F] T
pc_perturbation 0.0050 [5d-3]

Thermodynamic options:

solvus_tolerance aut [aut] or 0->1; aut = automatic, 0 => p=c pseudocompounds, 1 => homogeniz
T_stop (K) 0.0 [0]
T_melt (K) 873.0 [873]
approx_alpha T [T] F
Anderson-Gruneisen F [F] T
speciation_precision 0.1E-4 [1d-5] <1; absolute
speciation_max_it 100 [100]
GFSM F [F] T GFSM/special_component toggle
hybrid_EoS_H2O 4 [4] 0-2, 4-7
hybrid_EoS_CO2 4 [4] 0-4, 7
hybrid_EoS_CH4 0 [0] 0-1, 7
aq_bad_results err [err] 101 102 103 ignore
aq_lagged_speciation F [F] T
aq_ion_H+ T [T] F => use OH-
aq_oxide_components F [F] T
aq_solvent_solvus T [T] F
aq_vapor_epsilon 1.0 [1.]

Input/Output options:

pause_on_error T [T] F
timing T [T] F
auto_exclude T [T] F

To change these options see: www.perplex.ethz.ch/perplex_options.html

Summary of make-definition entities:

fbr fchum fphA fatg atgts cumm_dqf grun_dqf fanth_dq ged_dqf sil8L fo8L fa8L q8L cfs cenjh
qjL fojL fajL foTL faTL cfsg mfpv cmpv cfpv capv fcor hmgts foHL faHL qHL

Summary of saturated-component entities:

for: SiO2

q trd crst coe stv qL
q8L qjL qHL

for: SiO2 MU

mu

*solutions may also have compositions consisting entirely of saturated components

****warning ver013**** because the total amount of the components in san is <= 0, it will be rejected from this calculation. To prevent its rejection transform the data base components so that the total amount of the components in san is > 0.

Solution model summary:

****warning ver114**** the following endmembers are missing for Chl(W)

mnchl ff3cli f3clin

****warning ver101**** eliminated subcomposition [Mn][Mn] during reformulation of Chl(W) due to missing endme

****warning ver102**** reformulated subcomposition [M][M,T] of Chl(W) due to missing endmembers.

3074 pseudocompounds generated for: Chl(W)

****warning ver114**** the following endmembers are missing for Gt(W)

sps gr fmn_i fkho_i kho1 andr_i

****warning ver050**** reformulating prismatic solution: Gt(W) because of missing endmembers.
(reformulation can be controlled explicitly by excluding additional endmembers).

16 pseudocompounds generated for: Gt(W)

****warning ver114**** the following endmembers are missing for Ctd(W)

ctdo mnctd

16 pseudocompounds generated for: Ctd(W)

****warning ver114**** the following endmembers are missing for St(W)

mstt msto mnst

****warning ver102**** reformulated subcomposition X_Mg of St(W) due to missing endmembers.

16 pseudocompounds generated for: St(W)

****warning ver114**** the following endmembers are missing for Bi(W)

mnbi ffb_i_d fbi ftbi_d tbi

****warning ver101**** eliminated subcomposition [Mn][Mn] during reformulation of Bi(W) due to missing endme

****warning ver102**** reformulated subcomposition [M,T][M] of Bi(W) due to missing endmembers.

100 pseudocompounds generated for: Bi(W)

****warning ver114**** the following endmembers are missing for Crd(W)

mnocrd hmncrd_i

****warning ver050**** reformulating prismatic solution: Crd(W) because of missing endmembers.
(reformulation can be controlled explicitly by excluding additional endmembers).

286 pseudocompounds generated for: Crd(W)

Total number of pseudocompounds: 3508

Summary of included solution models:

Chl(W) Gt(W) Ctd(W) St(W) Bi(W) Crd(W)

**** Starting exploratory computational stage ***

Computing the compositional phase relations at condition 1

cycle 1 1 1

cycle 2 2 2

...

...

Computing the compositional phase relations at condition 2

cycle 1 1 1

cycle 2 2 2

...

...

Computing the compositional phase relations at condition 3

cycle 1 1 1

cycle 2 2 2

...

...

Computing the compositional phase relations at condition 4

cycle 1 1 1

cycle 2 2 2

...

...

****warning ver991**** The following solutions have compositions at an internal limit (i.e., $0 < x < 1$):

St(W)

Restriction during the auto-refine stage is usually unimportant. If desired, confirm by comparing the ranges below to those in the *.arf file.

NOTE: unintentional restrictions encountered during the exploratory stage may be problematic, refer to the *_auto_refine.txt file for the exploratory stage warnings.

Compositions for prismatic model: Chl(W)

Simplex 1

	Minimum	Maximum
X_Mames	0.11025	0.41650
X_Mafchl	0.0000	0.0000
X_Mclin	0.58350	0.88975

Simplex 2

	Minimum	Maximum
X_Mg	0.0000	0.60638
X_Fe	0.39362	1.0000

Compositions for simplicial model: Gt(W)

	Minimum	Maximum
alm	0.87419	0.99731
py	0.26875E-02	0.12581

Compositions for simplicial model: St(W)

	Minimum	Maximum
X_mst	0.31250E-03	0.42106
X_fst	0.57894	0.99969

Compositions for prismatic model: Bi(W)

Simplex 1

	Minimum	Maximum
X_Mg	0.0000	1.0000
X_Fe	0.0000	1.0000

Simplex 2

	Minimum	Maximum
X_AITs	0.0000	0.26119
X_MBio	0.73881	1.0000

The failure rate during speciation (order-disorder) calculations is 0.000% out of a total of 354350. calculations.

Average number of iterations per speciation calculation: 4.5

(3) Plotting the calculated phase diagram (PSVDRAW)

Run PSVDRAW to plot the calculated pseudosection:

```
C:\PERPLEX\Perplex691>psvdraw
```

Perple_X version 6.9.1, source updated January 3, 2022.

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Enter the project or plot file name [i.e., without the .plt suffix]:

ex8

Perple_X plot options are currently set as:

```
Keyword:      Value:  Permitted values [default]:
axis_label_scale  1.20  [1.2] (rel)
bounding_box :
    0  [0] x-min (pts)
    0  [0] y-min (pts)
    800 [800] x-length (pts)
    800 [800] y-length (pts)
field_fill      T  [T] F
field_label     T  [T] F
numeric_field_label F  [F] T, if T PSSECT writes list to *_assemblages.txt
replicate_label 0.250 0->1 [0.025]
field_label_scale 0.75  [0.72] (rel)
font            Helvetica
grid           F  [F] T
half_ticks     T  [T] F
line_width     1.00  0-99 [1.] (pts)
picture_transformation :
    0.180 [0.18] x-scale (rel)
    0.180 [0.18] y-scale (rel)
    130.  [0.18] x-translation (pts)
    220.  [0.18] y-translation (pts)
    0.00  [0.0] rotation (deg)
plot_aspect_ratio 1.000 [1.0] x_axis_length/y_axis_length
splines          T  [T] F
tenth_ticks     F  [F] T
text_scale      1.000 [1.] (rel)
plot_extra_data
```

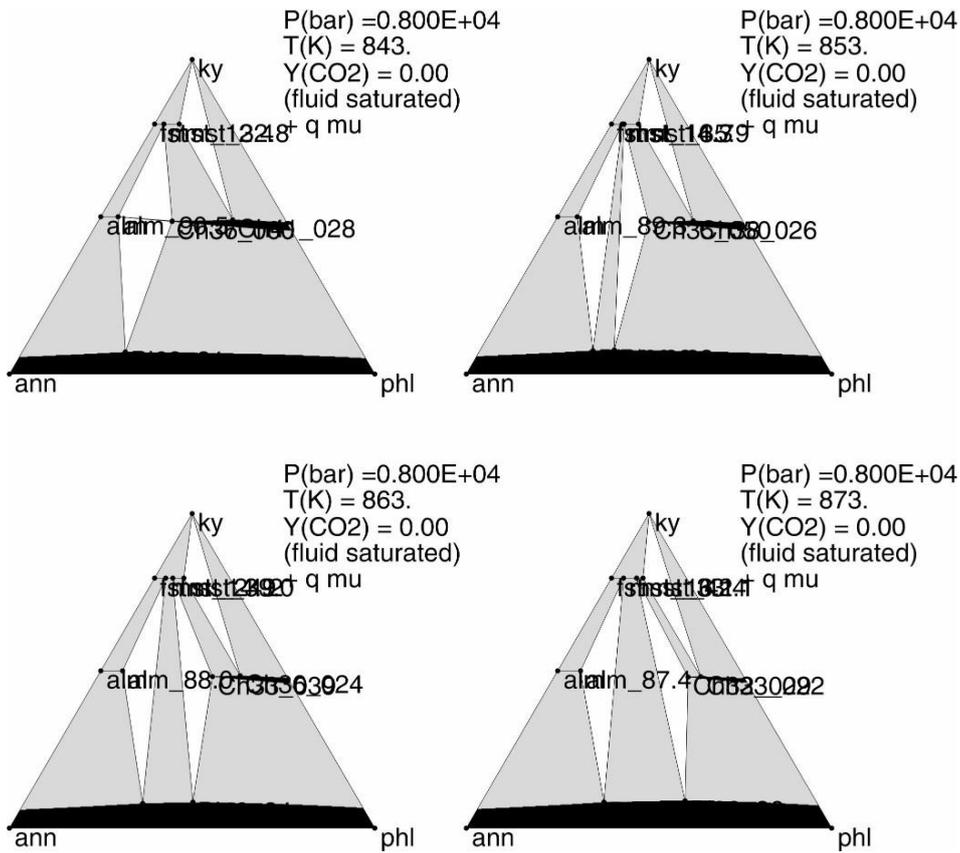
To change these options edit or create the plot option file

See: www.perplex.ethz.ch/perplex_plot_options.html

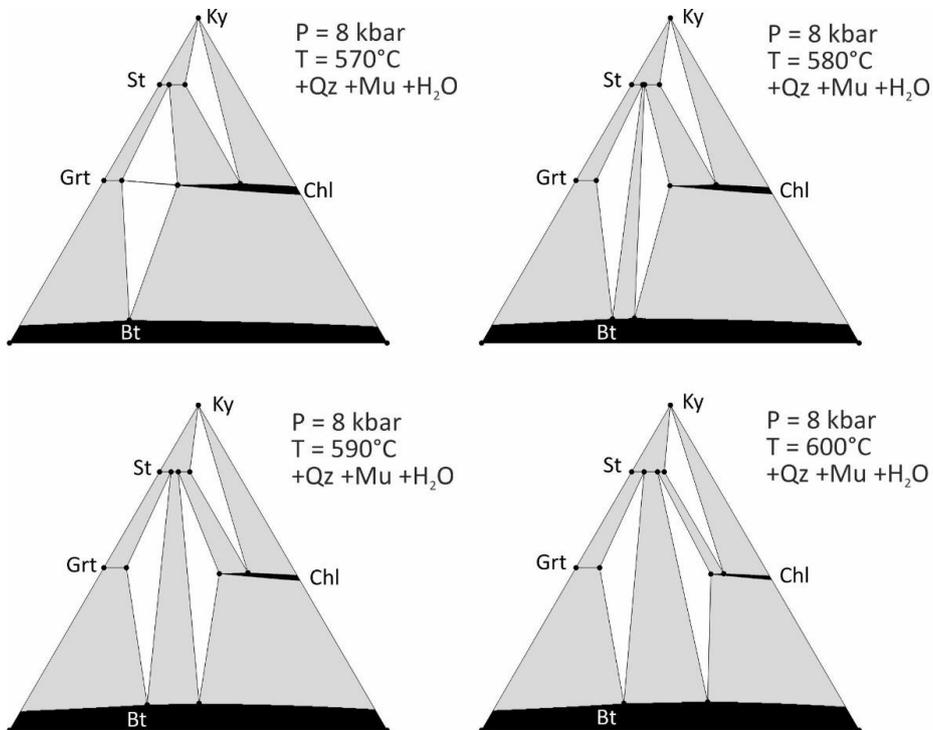
PostScript will be written to file: ex8.ps

Modify the default plot (y/n)?

n



In the resulting diagrams white fields are three-phases fields (+Qz+Mu+H2O), grey fields are two-phases fields (+Qz+Mu+H2O) and black fields are one-phase fields (+Qz+Mu+H2O).



The AFM diagrams predict the stable mineral assemblages and compositions at specific P-T conditions, as a function of the bulk rock composition.

Ex 9

Ex. 9 – P-T pseudosection for a METAPELITE in the KFMASH system

This exercise explains how to calculate a P-T pseudosection for a metapelite sample, in the simplified KFMASH system. The problem is a bit more complex than Ex. 4, because it involves **SOLID SOLUTIONS**. The influence of other components (Na₂O, CaO and MnO) will be considered in the next exercise (Ex. 10). At the end, some practical tips for redrawing the PerpleX outputs are given, and the comparison with the AFM chemographies calculated in Ex. 8 will be done.

This exercise also explains how to calculate **compositional ISOPLETHS** and **ISOMODES**.

The exercise is based on the paper by Tinkham et al. (2001) [Geol. Mat. Res., 3, 1-42]. The modelled sample is AWBZ (see Table 1 and their Fig. 3).

Total bulk composition (mol%; SiO₂ in excess):

Al₂O₃=37.99, FeO=21.93, MgO=19.59, MnO=0.42, CaO=4.95, Na₂O=6.11, K₂O=9.01

Bulk composition recalculated ignoring MnO, CaO and Na₂O components:

Al₂O₃=42.92, FeO=24.77, MgO=22.13, K₂O=10.18

T=425-700°C

P=1-10 kbar

(1) Definition of the problem (BUILD)

```
C:\PERPLEX\Perplex691>build
```

Perple_X version 6.9.1, source updated January 3, 2022.

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NO is the default (blank) answer to all Y/N prompts

Enter a name for this project (the name will be used as the root for all output file names) [default = my_project]:

ex9

The problem definition file will be named: ex9.dat

Enter thermodynamic data file name [default = hp02ver.dat]:

hp62ver.dat

Enter the computational option file name [default = perplex_option.dat]:

See: www.perplex.ethz.ch/perplex_options.html

[enter]

Reading Perple_X options from: perplex_option.dat

The current data base components are:

Na2O MgO Al2O3 SiO2 K2O CaO TiO2 MnO FeO NiO ZrO2 Cl2 O2 H2O CO2 CuO Cr2O3 S2 F2 N2
Transform them (Y/N)?

n

Specify computational mode:

- 1 - Convex-Hull minimization
- 2 - Constrained minimization on a 2d grid [default]
- 3 - Constrained minimization on a 1d grid
- 4 - Output pseudocompound data
- 5 - 1-d Phase fractionation
- 6 - 0-d Infiltration-reaction-fractionation
- 7 - 2-d Phase fractionation (FRAC2D and TITRATE reactive transport models)

Use Convex-Hull minimization for Schreinemakers projections or phase diagrams with > 2 independent variables. Use constrained minimization for phase diagrams or phase diagram sections with < 3 independent variables.

2

Calculations with a saturated fluid (Y/N)?

y

Select the independent saturated fluid components:

H2O CO2

Enter names, 1 per line, press <enter> to finish:

For C-O-H fluids it is only necessary to select volatile species present in the solids of interest. If the species listed here are H2O and CO2, then to constrain O2 chemical potential to be consistent with C-O-H fluid speciation treat O2 as a saturated component. Refer to the Perple_X Tutorial for details.

H2O

Calculations with saturated components (Y/N)?

y

****warning ver015**** if you select > 1 saturated component, then the order you enter the components determines the saturation heirarchy and may effect your results (see Connolly 1990).

Select < 6 saturated components from the set:

Na2O MgO Al2O3 K2O CaO TiO2 MnO FeO NiO ZrO2 Cl2 O2 CO2 CuO Cr2O3 S2 F2 N2

Enter names, 1 per line, press <enter> to finish:

SiO2

Use chemical potentials, activities or fugacities as independent variables (Y/N)?

n

Select thermodynamic components from the set:

Na2O MgO Al2O3 K2O CaO TiO2 MnO FeO NiO ZrO2 Cl2 O2 CO2 CuO Cr2O3 S2 F2 N2

Enter names, 1 per line, press <enter> to finish:

MgO

Al2O3

K2O

FeO

Because the thermodynamic data file identifies: H2O as special components, you will be prompted next for the EoS to be used for the corresponding components and mixtures thereof. To override this behavior, e.g., to use a generic hybrid fluid EoS, delete the special_component section from the thermodynamic data file header.

NOTE: the EoS choice specified here will override the EoS choice specified by the hybrid_EoS option, to override this behavior delete the special_component section from the the thermodynamic data file header.

Select fluid equation of state:

- 0 - X(CO2) H2O-CO2 Modified Redlich-Kwong (MRK) DeSantis et al 74
- 1 - X(CO2) H2O-CO2 HSMRK Kerrick & Jacobs 81
- 2 - X(CO2) H2O-CO2 MRK hybrid-EoS*
- 5 - X(CO2) H2O-CO2 CORK Holland & Powell 91, 98
- 8 - f(O2/CO2) C-buffered COH MRK hybrid-EoS*
- 10 - X(O) C-buffered COH MRK hybrid-EoS Connolly & Cesare 93*
- 12 - X(O)-f(S2) C-buffered COHS MRK hybrid-EoS Connolly & Cesare 93*
- 13 - X(H2) H2O-H2 MRK hybrid-EoS*
- 14 - X(CO2) H2O-CO2 Pitzer & Sterner 94; Holland & Powell mixing 03
- 15 - X(H2) H2O-H2 low T MRK hybrid-EoS*
- 16 - X(O) H-O MRK hybrid-EoS*
- 17 - X(O)-f(S2) H-O-S MRK hybrid-EoS*
- 19 - X(O)-X(S) C-buffered COHS MRK hybrid-EoS Connolly & Cesare 93*
- 20 - X(O)-X(C) COHS MRK hybrid-EoS Connolly & Cesare 93*
- 24 - f(O2/CO2)-N/C C-buffered COHN MRK hybrid-EoS*
- 25 - X(CO2)-X(NaCl) H2O-CO2-NaCl Aranovich et al 10
- 26 - X(O) O-Si MRK Connolly 16
- 27 - X(O)-X(C) C-O-H MRK hybrid-EoS*

*Hybrid EoS use the following pure species EoS, to change these associations modify the hybrid_EoS keywords in the perplex_option file:

- H2O - PSEoS Pitzer & Sterner 1994
- CO2 - PSEoS Pitzer & Sterner 1994
- CH4 - MRK DeSantis et al 1974

5

The data base has P(bar) and T(K) as default independent potentials.

Make one dependent on the other, e.g., as along a geothermal gradient (y/n)?

n

Select x-axis variable:

- 1 - P(bar)
- 2 - T(K)
- 3 - Y(CO2)
- 4 - Composition X_C1* (user defined)

*Although only one component is specified for the Y(CO2) phase, its equation of state permits use of its compositional variable:

*X_C1 can not be selected as the y-axis variable

2

Enter minimum and maximum values, respectively, for: T(K)

698

973

Select y-axis variable:

2 - P(bar)

3 - Y(CO2)

2

Enter minimum and maximum values, respectively, for: P(bar)

1000

10000

Specify sectioning value for: Y(CO2)

0

For gridded minimization, grid resolution is determined by the number of levels (grid_levels) and the resolution at the lowest level in the X- and Y-directions (x_nodes and y_nodes) these parameters are currently set for the exploratory and autorefine cycles as follows:

stage	grid_levels	xnodes	ynodes	effective resolution
-------	-------------	--------	--------	----------------------

exploratory	1	40	40	40 x 40 nodes
-------------	---	----	----	---------------

auto-refine	4	60	60	473 x 473 nodes
-------------	---	----	----	-----------------

To change these options edit or create the file perplex_option.dat

See: www.perplex.ethz.ch/perplex_options.html#grid_parameters

All thermodynamic components must be constrained, specify saturated components also (Y/N)?

n

Specify component amounts by mass (Y/N)?

n

The amounts you enter next need not be normalized; regardless of units, they define the molar amount of the system

Enter the molar amounts of the components:

MgO Al2O3 K2O FeO

for the bulk composition of interest:

22.13

42.92

10.18

24.77

Output a print file (Y/N)?

y

Exclude pure and/or endmember phases (Y/N)?

n

Include solution models (Y/N)?

Y

Enter the solution model file name [default = solution_model.dat]:

[enter]

...

Select models from the following list, enter 1 per line, press <enter> to finish

clinoamphibole models: cAmph_I(G) cAmph(G) Cumm cAmph(DP) cAmph_I(DP)

clinopyroxene models: Cpx_I(HGP) Cpx(HGP) Augite(G) Cpx(JH)...

...

For details on these models see: www.perplex.ethz.ch/perplex_solution_model_glossary.html or read the commentary in the solution model file.

Chl(W)

Bi(W)

Gt(W)

Ctd(W)

St(W)

Crd(W)

Enter calculation title:

Ex8

(2) Doing the calculation (VERTEX)

Run VERTEX to make the calculation:

```
C:\PERPLEX\Perplex691>vertex
```

Perple_X version 6.9.1, source updated January 3, 2022.

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Enter the project name (the name assigned in BUILD) [default = my_project]:

ex9

Reading problem definition from file: ex9.dat

Reading thermodynamic data from file: hp62ver.dat

Writing print output to file: ex9.plt

Writing plot output to file: ex9.plt

Writing phase assemblage data to file: ex9.blk

Reading solution models from file: solution_model.dat

Reading Perple_X options from: perplex_option.dat

Writing auto refine summary to: not requested

Writing seismic data options to: ex9_seismic_data.txt

Writing pseudocompound glossary to: ex9_pseudocompound_glossary.txt

Writing Perple_X option summary to: not requested

Perple_X computational option settings for VERTEX:

Keyword: Value: Permitted values [default]:

Auto-refine options:

auto_refine aut [auto] manual off

replicate_threshold 0.1E-1 [1e-2]; static opt; <0 => no replica test

rep_dynamic_threshold 0.1E-2 [1d-3]; dynamic opt; <0 => no replica test

re-refine F [F] T

intermediate_savrpc F [F] T
intermediate_savdyn F [F] T
keep_all_rpc T [T] F

Free energy minimization options:

MINFRC_diff_increment 0.1E-6 [1e-7] 1e-3 => 1e-9
MINFXC_solver 0 [0] >= 0 - speci2, -1 - MINFXC
optimization_max_it 40 [40] >1
optimization_precision 0.1E-3 [1e-4], 1e-1 => 1e-6, absolute
order_check F [F] T
refinement_points 6 [auto] 1->14
refinement_switch F [T] F
scatter-points T [T] F
scatter-increment 0.1E-1 [1e-2] 1e-2 => 1e-7
solvus_tolerance_ll aut [0.2] 0->1
zero_mode 0.1E-5 [1e-6] 0->1; < 0 => off

2D grid options:

x_nodes 40 / 60 [10/40] >0, <2048; effective x-resolution 40 / 473 nodes
y_nodes 40 / 60 [10/40] >0, <2048; effective y-resolution 40 / 473 nodes
grid_levels 1 / 4 [1/4] >0, <10
linear_model on [on] off

Solution subdivision options:

initial_resolution: 0.2500 [1/4] 0->1; 0 => off
stretch_factor 0.0020 [2d-3] >0
non_linear_switch F [F] T
subdivision_override off [lin] off str
refine_endmembers F [F] T

Thermodynamic options:

solvus_tolerance aut [aut] or 0->1; aut = automatic, 0 => p=c pseudocompounds, 1 => homogenize
T_stop (K) 0.0 [0]
T_melt (K) 873.0 [873]
approx_alpha T [T] F
Anderson-Gruneisen F [F] T
speciation_precision 0.1E-4 [1d-5] <1; absolute
speciation_max_it 100 [100]
GFSM F [F] T GFSM/special_component toggle
hybrid_EoS_H2O 4 [4] 0-2, 4-7
hybrid_EoS_CO2 4 [4] 0-4, 7
hybrid_EoS_CH4 0 [0] 0-1, 7
aq_bad_results err [err] 101 102 103 ignore
aq_lagged_speciation F [F] T
aq_ion_H+ T [T] F => use OH-
aq_oxide_components F [F] T
aq_solvent_solvus T [T] F
aq_vapor_epsilon 1.0 [1.]

Input/Output options:

pause_on_error T [T] F
timing T [T] F
auto_exclude T [T] F
logarithmic_p F [F] T
bad_number NaN [NaN]
interim_results aut [auto] off manual

Information file output options:

option_list_files F [F] T; echo computational options
pseudocompound_file T [F] T; echo static pseudocompound compositions
auto_refine_file F [T] F; echo auto-refine compositions
seismic_data_file T [F] T; echo seismic wavespeed options

To change these options see: www.perplex.ethz.ch/perplex_options.html

Summary of make-definition entities:

fbr fchum fphA fatg atgts cumm_dqf grun_dqf fanth_dq ged_dqf sil8L fo8L fa8L q8L cfs
cenjh qjL fojL fajL foTL faTL cfsq mfpv cmpv cfpv capv fcor hmgts kjdh foHL faHL
qHL kjL

Summary of saturated-component entities:

for: SiO2

q trd crst coe stv qL
q8L qjL qHL

warning ver099 no data for aqueous species, aq_output and aq_lagged_speciation disabled.

Solution model summary:

warning ver114 the following endmembers are missing for Chl(W)

mnchl ff3cli f3clin

warning ver101 eliminated subcomposition [Mn][Mn] during reformulation of Chl(W) due to missing endmembers.

warning ver102 reformulated subcomposition [M][M,T] of Chl(W) due to missing endmembers.

71 pseudocompounds generated for: Chl(W)

warning ver114 the following endmembers are missing for Gt(W)

spss gr fmn_i fkho_i kho1 andr_i

warning ver050 reformulating prismatic solution: Gt(W) because of missing endmembers.
(reformulation can be controlled explicitly by excluding additional endmembers).

3 pseudocompounds generated for: Gt(W)

warning ver114 the following endmembers are missing for Ctd(W)

ctdo mnctd

3 pseudocompounds generated for: Ctd(W)

warning ver114 the following endmembers are missing for St(W)

mstt msto mnst

warning ver102 reformulated subcomposition X_Mg of St(W) due to missing endmembers.

3 pseudocompounds generated for: St(W)

warning ver114 the following endmembers are missing for Bi(W)

mnbi ffb_i_d fbi ftbi_d tbi

warning ver101 eliminated subcomposition [Mn][Mn] during reformulation of Bi(W) due to missing endmembers.

warning ver102 reformulated subcomposition [M,T][M] of Bi(W) due to missing endmembers.

13 pseudocompounds generated for: Bi(W)

warning ver114 the following endmembers are missing for Crd(W)

mnocrd hmncrd_i

warning ver050 reformulating prismatic solution: Crd(W) because of missing endmembers.
(reformulation can be controlled explicitly by excluding additional endmembers).

22 pseudocompounds generated for: Crd(W)

Total number of pseudocompounds: 115

Summary of included solution models:

Chl(W) Gt(W) Ctd(W) St(W) Bi(W) Crd(W)

This is the beginning of the EXPLORATORY COMPUTATIONAL STAGE

2.4% done with low level grid.
4.9% done with low level grid.
7.3% done with low level grid.
9.8% done with low level grid.
12.2% done with low level grid.
14.6% done with low level grid.
17.1% done with low level grid.
19.5% done with low level grid.
22.0% done with low level grid.
24.4% done with low level grid.
26.8% done with low level grid.
29.3% done with low level grid.
31.7% done with low level grid.
34.1% done with low level grid.
36.6% done with low level grid.
39.0% done with low level grid.
41.5% done with low level grid.
43.9% done with low level grid.
46.3% done with low level grid.
48.8% done with low level grid.
51.2% done with low level grid.
53.7% done with low level grid.
56.1% done with low level grid.
58.5% done with low level grid.
61.0% done with low level grid.
63.4% done with low level grid.
65.9% done with low level grid.
68.3% done with low level grid.
70.7% done with low level grid.
73.2% done with low level grid.
75.6% done with low level grid.
78.0% done with low level grid.
80.5% done with low level grid.
82.9% done with low level grid.
85.4% done with low level grid.
87.8% done with low level grid.
90.2% done with low level grid.
92.7% done with low level grid.
95.1% done with low level grid.
97.6% done with low level grid.

Exploratory stage generated:

262 compositions for: Chl(W)

17 compositions for: Gt(W)

10 compositions for: Ctd(W)

27 compositions for: St(W)
535 compositions for: Bi(W)
167 compositions for: Crd(W)
Total number of compositions: 1018

This is the beginning of the AUTO-REFINE STAGE

** Starting auto-refine computational stage **

1.7% done with low level grid.
3.3% done with low level grid.
5.0% done with low level grid.
6.7% done with low level grid.
8.3% done with low level grid.
10.0% done with low level grid.
11.7% done with low level grid.
13.3% done with low level grid.
15.0% done with low level grid.
16.7% done with low level grid.
18.3% done with low level grid.
20.0% done with low level grid.
21.7% done with low level grid.
23.3% done with low level grid.
25.0% done with low level grid.
26.7% done with low level grid.
28.3% done with low level grid.
30.0% done with low level grid.
31.7% done with low level grid.
33.3% done with low level grid.
35.0% done with low level grid.
36.7% done with low level grid.
38.3% done with low level grid.
40.0% done with low level grid.
41.7% done with low level grid.
43.3% done with low level grid.
45.0% done with low level grid.
46.7% done with low level grid.
48.3% done with low level grid.
50.0% done with low level grid.
51.7% done with low level grid.
53.3% done with low level grid.
55.0% done with low level grid.
56.7% done with low level grid.
58.3% done with low level grid.
60.0% done with low level grid.
61.7% done with low level grid.
63.3% done with low level grid.
65.0% done with low level grid.
66.7% done with low level grid.
68.3% done with low level grid.
70.0% done with low level grid.
71.7% done with low level grid.

73.3% done with low level grid.
 75.0% done with low level grid.
 76.7% done with low level grid.
 78.3% done with low level grid.
 80.0% done with low level grid.
 81.7% done with low level grid.
 83.3% done with low level grid.
 85.0% done with low level grid.
 86.7% done with low level grid.
 88.3% done with low level grid.
 90.0% done with low level grid.
 91.7% done with low level grid.
 93.3% done with low level grid.

warning ver106 chemical potentials could not be determined after 8 iterations.

Iteration has been aborted and the low quality result output.

Current conditions:

T(K) = 959.0169
 P(bar) = 2830.508
 Y(CO2) = 0.000000

95.0% done with low level grid.
 96.7% done with low level grid.
 98.3% done with low level grid.
 100.0% done with low level grid.

Beginning grid refinement stage.

588 grid cells to be refined at grid level 2
 ...working (501 minimizations done)
 ...working (1002 minimizations done)
 refinement at level 2 involved 1253 minimizations
 4853 minimizations required of the theoretical limit of 14161

1044 grid cells to be refined at grid level 3
 ...working (252 minimizations done)
 ...working (753 minimizations done)
 ...working (1254 minimizations done)
 ...working (1757 minimizations done)
 refinement at level 3 involved 1909 minimizations
 6762 minimizations required of the theoretical limit of 56169

1767 grid cells to be refined at grid level 4
 ...working (349 minimizations done)
 ...working (851 minimizations done)
 ...working (1352 minimizations done)
 ...working (1853 minimizations done)
 ...working (2355 minimizations done)
 ...working (2857 minimizations done)
 refinement at level 4 involved 2961 minimizations
 9723 minimizations required of the theoretical limit of 224676

Timing	min.	% of total
Static G calculation	0.37180	18.5
Dynamic G calculation	0.62322	31.0
Static LP	0.98801E-02	0.5

Dynamic LP	0.40300E-01	2.0
Successive QP	0.93627	46.6
Total of above	1.9815	98.5
Total elapsed time	2.0111	100.0

End of job: ex9

At the end of the calculation, a number of new files appear in the Perple_X folder. The most useful are the *****.prn** and the *****.plt** files (i.e. the text file and the plot file).

(3) Plotting the calculated phase diagram (PSSECT)

Run PSSECT to plot the calculated pseudosection:

C:\PERPLEX\Perplex691>pssect

Perple_X version 6.9.1, source updated January 3, 2022.

Copyright (C) 1986-2022 James A D Connolly <www.perplex.ethz.ch/copyright.html>.

Enter the project name (the name assigned in BUILD) [default = my_project]:

ex9

Reading Perple_X options from: perplex_option.dat

Perple_X plot options are currently set as:

Keyword:	Value:	Permitted values [default]:
axis_label_scale	1.20	[1.2] (rel)
bounding_box :		
	0	[0] x-min (pts)
	0	[0] y-min (pts)
	800	[800] x-length (pts)
	800	[800] y-length (pts)
field_fill	T	[T] F
field_label	T	[T] F
numeric_field_label	F	[F] T, if T PSSECT writes list to *_assemblages.txt
replicate_label	0.250	0->1 [0.025]
field_label_scale	0.75	[0.72] (rel)
font	Helvetica	
grid	F	[F] T
half_ticks	T	[T] F
line_width	1.00	0-99 [1.] (pts)
picture_transformation :		
	0.180	[0.18] x-scale (rel)
	0.180	[0.18] y-scale (rel)
	130.	[0.18] x-translation (pts)
	220.	[0.18] y-translation (pts)
	0.00	[0.0] rotation (deg)
plot_aspect_ratio	1.000	[1.0] x_axis_length/y_axis_length
splines	T	[T] F

```
tenth_ticks      F      [F] T
text_scale       1.000  [1.] (rel)
plot_extra_data
```

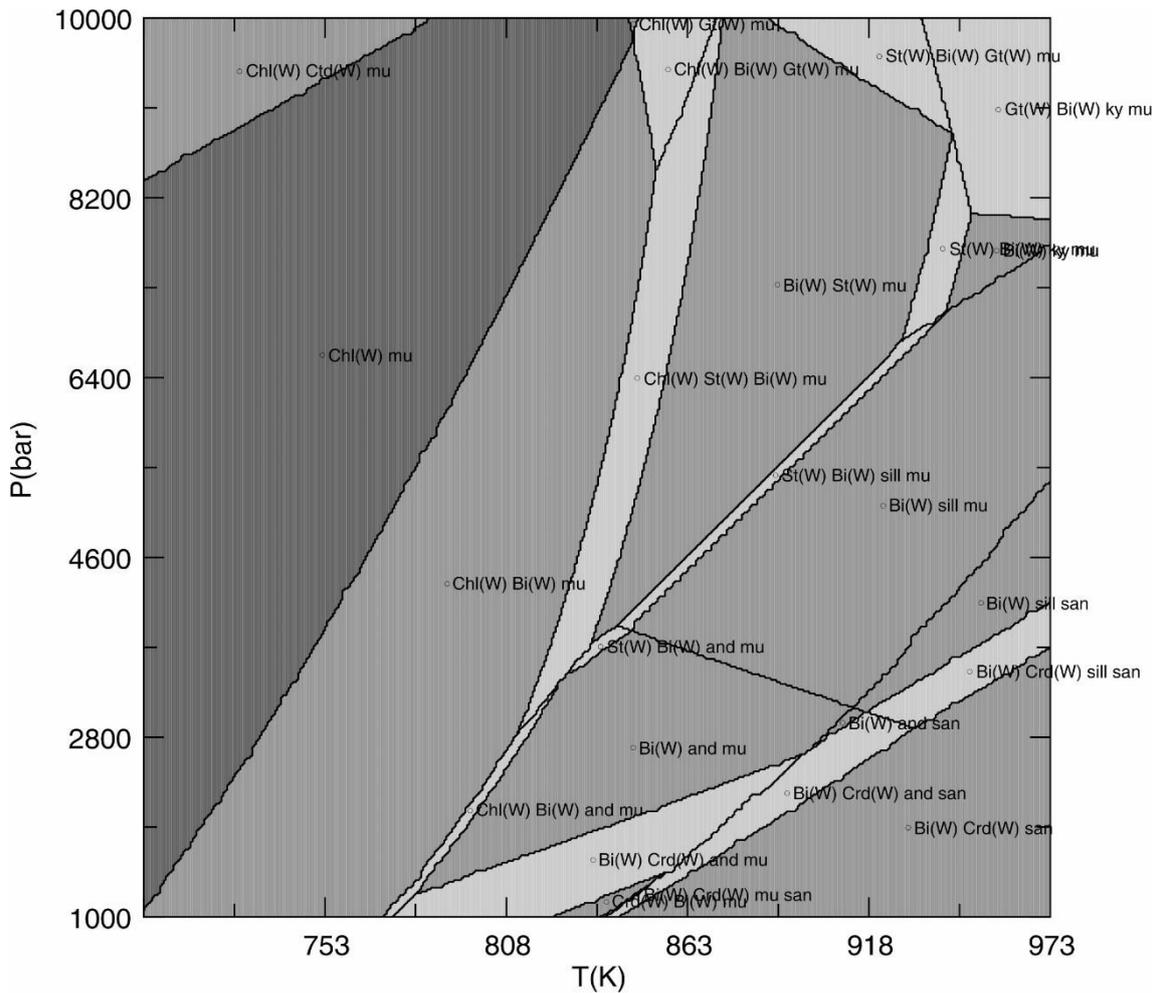
To change these options edit or create the plot option file
 See: www.perplex.ethz.ch/perplex_plot_options.html

PostScript will be written to file: ex9.ps

Modify the default plot (y/n)?

n

There are 5 fields for: Bi(W) Crd(W) mu san



Quartz and H₂O are in excess.

In the calculated pseudosection, field assemblages have different variances. Fields with the same grey colour have the same variance. Colour code is as follows: light grey = 2-variant fields (6 phases), medium grey = 3-variant fields (5 phases), dark grey = 4-variant fields (4 phases). Darker is the colour, higher is the variance (and lower is the number of phases!).

(4) PRACTICAL TIPS FOR RE-DRAWING THE PERPLE_X OUTPUTS

In most cases, you should re-draw the final output in order to obtain a result that can be published. When re-drawing a pseudosection, be careful to not introduce topological errors.

General rules are:

(1) Fields with the same variance should be indicated with the same colour.

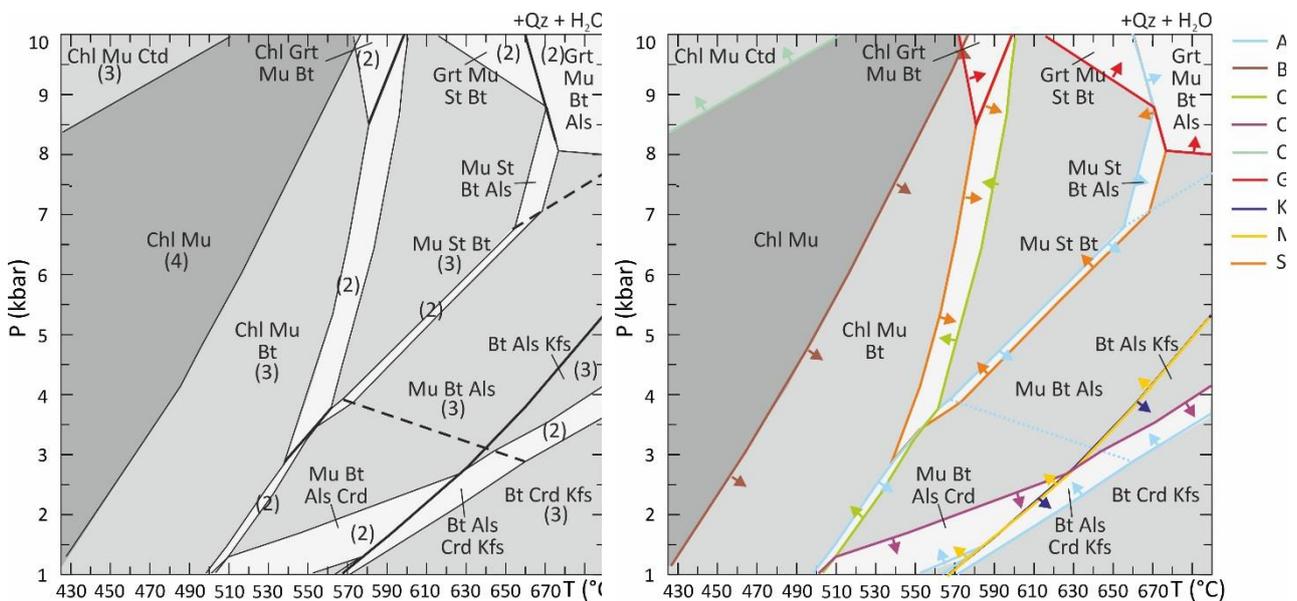
Remember that: $F = C - P + 2$. In this case: $C = 6$ (KFMASH)

Therefore, fields characterized by 6 phases ($P=6$; light grey fields in the pseudosection) are divariant ($F=6-6+2$); fields with 5 phases (medium grey) are tri-variant and so on.

(2) in a point cannot converge more than 4 lines

(3) 2 fields with the same variance n (i.e. with the same n° of phases) are always separated by a $(n+1)$ or $(n-1)$ -variant field, except when they are separated by a true univariant curve.

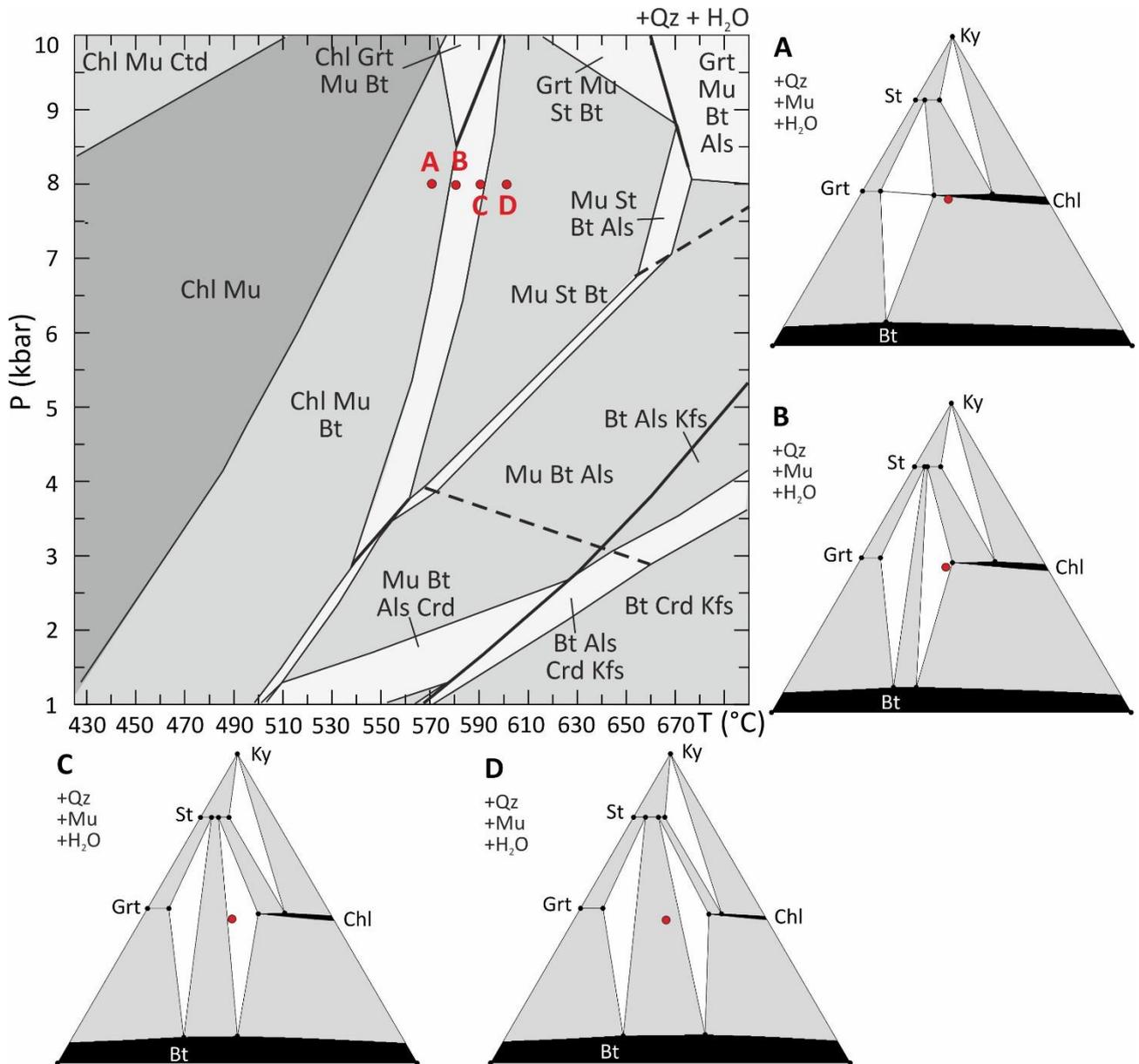
(4) Lines between fields always mark the APPEARANCE or DISAPPEARANCE of a phase



In the diagram on the left, variance of each field is reported in brackets. The thick black lines are true univariant reactions.

In the diagram on the right, the phase-in boundaries are reported with different colours for each phase.

(5) COMPARISON BETWEEN AFM DIAGRAMS AND PSEUDOSECTION



Comparison between AFM diagrams (Ex.8) calculated at P-T conditions A to D and the pseudosection calculated in the KFMASH system (Ex. 9) for a bulk composition $K_2O=10.18$, $FeO=24.77$, $MgO=22.13$, $Al_2O_3=42.92$ mol% (red dot in the AFM diagrams).

Mineral assemblages predicted by AFM diagrams for this specific bulk rock composition (red dot) must correspond to the assemblages predicted by the P-T pseudosection at the same P-T conditions.

(6) Calculating ISOMODES (WERAMI)

This section explains how to calculate the variation in the modal amounts of each mineral phase (vol%), for the modelled pseudosection.

```
C:\PERPLEX\Perplex691>werami
```

Perple_X version 6.9.1, source updated January 14, 2022.

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Enter the project name (the name assigned in BUILD) [default = my_project]:

```
ex9
```

Reading Perple_X options from: perplex_option.dat

Writing Perple_X option summary to: not requested

Perple_X computational option settings for WERAMI:

Keyword: Value: Permitted values [default]:

Input/Output options:

```
aqueous_output      T      [F] T
aqueous_species     20     [20] 0-150
aq_solvent_composition y      [y] m: y => mol fraction, m => molality
aq_solute_composition m      y [m]: y => mol fraction, m => molality
spreadsheet         T      [F] T
logarithmic_p       F      [F] T
bad_number          NaN    [NaN]
composition_constant F      [F] T
composition_phase   mol    [mol] wt
composition_system   wt    [wt] mol
proportions         vol    [vol] wt mol
absolute            F      [F] T
cumulative          F      [F] T
fancy_cumulative_modes F      [F] T
interpolation       on     [on] off
melt_is_fluid       F      [F] T
solution_names      mod    [model] abbreviation full
structural_formulae T      [T] F
output_species      T      [T] F
output_species_props F      [F] T
seismic_output      som    [some] none all
pause_on_error      T      [T] F
poisson_test        F      [F] T
interim_results     aut    [auto] off manual
sample_on_grid      T      [T] F
auto_exclude        T      [T] F
```

Information file output options:

```
option_list_files   F      [F] T; echo computational options
```

Thermodynamic options:

```
approx_alpha       T      [T] F
```

Anderson-Gruneisen F [F] T
 hybrid_EoS_H2O 4 [4] 0-2, 4-7
 hybrid_EoS_CO2 4 [4] 0-4, 7
 hybrid_EoS_CH4 0 [0] 0-1, 7
 fd_expansion_factor 2.0 [2] >0
 finite_difference_p 0.1E+05 [1d4] >0; fraction = 0.1E-02 [1d-2]

Seismic wavespeed computational options:

seismic_data_file T [F] T
 bounds VRH [VRH] HS
 vrh/hs_weighting 0.5 [0.5] 0->1
 explicit_bulk_modulus T [T] F
 poisson_ratio on [on] all off; Poisson ratio = 0.35
 seismic_output som [some] none all
 poisson_test F [F] T
 Tisza_test F [F] T

To change these options see: www.perplex.ethz.ch/perplex_options.html

 Select operational mode:

- 1 - properties at specified conditions
- 2 - properties on a 2d grid
- 3 - properties along a 1d path
- 4 - as in 3, but input from file
- 0 - EXIT

2

Select a property:

- 1 - Specific Enthalpy (J/m³)
- 2 - Density (kg/m³)
- 3 - Specific heat capacity (J/K/m³)
- 4 - Expansivity (1/K, for volume)
- 5 - Compressibility (1/bar, for volume)
- 6 - Composition (Mol, Mass, or Wt%) of the system
- 7 - Mode (Vol, Mol, or Wt proportion) of a phase
- 8 - Composition (Mol, Mass, or Wt%) of a solution phase
- 9 - Grueneisen thermal ratio
- 10 - Adiabatic bulk modulus (bar)
- 11 - Adiabatic shear modulus (bar)
- 12 - Sound velocity (km/s)
- 13 - P-wave velocity (Vp, km/s)
- 14 - S-wave velocity (Vs, km/s)
- 15 - Vp/Vs
- 16 - Specific entropy (J/K/m³)
- 17 - Entropy (J/K/kg)
- 18 - Enthalpy (J/kg)
- 19 - Heat Capacity (J/K/kg)
- 20 - Specific mass of a phase (kg/m³-system)
- 21 - Poisson ratio
- 22 - Molar Volume (J/bar)
- 23 - Dependent potentials (J/mol, bar, K)
- 24 - Assemblage Index

- 25 - Modes of all phases
- 26 - Sound velocity T derivative (km/s/K)
- 27 - P-wave velocity T derivative (km/s/K)
- 28 - S-wave velocity T derivative (km/s/K)
- 29 - Adiabatic bulk modulus T derivative (bar/K)
- 30 - Shear modulus T derivative (bar/K)
- 31 - Sound velocity P derivative (km/s/bar)
- 32 - P-wave velocity P derivative (km/s/bar)
- 33 - S-wave velocity P derivative (km/s/bar)
- 34 - Adiabatic bulk modulus P derivative (unitless)
- 35 - Shear modulus P derivative (unitless)
- 36 - All phase &/or system properties
- 37 - Absolute amount (Vol, Mol, or Wt) of a phase
- 38 - Multiple property output
- 39 - Heat capacity ratio (Cp/Cv)
- 40 - Lagged or back-calculated aqueous solute chemistry

7

Enter solution or compound (left justified):

Gt(W)

Include fluid in computation of aggregate (or modal) properties (y/n)?

n

Fractions are Wt, Vol, or Mol depending on the perplex_option.dat proportions keyword.

Mode can be computed as vol%, mol% or wt%. The default value is vol%. You can control this parameter modifying the "proportions" keyword in the perplex_option.dat file

Select an additional property or enter 0 to finish:

7

Enter solution or compound (left justified):

ChI(W)

Include fluid in computation of aggregate (or modal) properties (y/n)?

n

Fractions are Wt, Vol, or Mol depending on the perplex_option.dat proportions keyword.

Select an additional property or enter 0 to finish:

7

Enter solution or compound (left justified):

Ctd(W)

Include fluid in computation of aggregate (or modal) properties (y/n)?

n

Fractions are Wt, Vol, or Mol depending on the perplex_option.dat proportions keyword.

Select an additional property or enter 0 to finish:

7

Enter solution or compound (left justified):

St(W)

Include fluid in computation of aggregate (or modal) properties (y/n)?

n

Fractions are Wt, Vol, or Mol depending on the perplex_option.dat proportions keyword.

Select an additional property or enter 0 to finish:

7

Enter solution or compound (left justified):

Bi(W)

Include fluid in computation of aggregate (or modal) properties (y/n)?

n

Fractions are Wt, Vol, or Mol depending on the perplex_option.dat proportions keyword.

Select an additional property or enter 0 to finish:

7

Enter solution or compound (left justified):

mu

Include fluid in computation of aggregate (or modal) properties (y/n)?

n

Fractions are Wt, Vol, or Mol depending on the perplex_option.dat proportions keyword.

Select an additional property or enter 0 to finish:

7

Enter solution or compound (left justified):

Crd(W)

Include fluid in computation of aggregate (or modal) properties (y/n)?

n

Fractions are Wt, Vol, or Mol depending on the perplex_option.dat proportions keyword.

Select an additional property or enter 0 to finish:

7

Enter solution or compound (left justified):

san

Include fluid in computation of aggregate (or modal) properties (y/n)?

n

Fractions are Wt, Vol, or Mol depending on the perplex_option.dat proportions keyword.

Select an additional property or enter 0 to finish:

7

Enter solution or compound (left justified):

ky

Include fluid in computation of aggregate (or modal) properties (y/n)?

n

Fractions are Wt, Vol, or Mol depending on the perplex_option.dat proportions keyword.

Select an additional property or enter 0 to finish:

7

Enter solution or compound (left justified):

sill

Include fluid in computation of aggregate (or modal) properties (y/n)?

n

Fractions are Wt, Vol, or Mol depending on the perplex_option.dat proportions keyword.

Select an additional property or enter 0 to finish:

7

Enter solution or compound (left justified):

and

Include fluid in computation of aggregate (or modal) properties (y/n)?

n

Fractions are Wt, Vol, or Mol depending on the perplex_option.dat proportions keyword.

Select an additional property or enter 0 to finish:

0

Change default variable range (y/n)?

n

Select the grid resolution (to use an arbitrary grid set sample_on_grid to F):

1 - 60 x 60 nodes

2 - 119 x 119 nodes

3 - 237 x 237 nodes

4 - 473 x 473 nodes [default]

4

...

...

Data ranges excluding values equal to bad_number (NaN) specified in perplex_option.dat:

	Gt(W),vo%	Chl(W),vo%	Ctd(W),vo%	St(W),vo%	Bi(W),vo%	mu,vo%	Crđ(W),vo%	san,vo%
ky,vo%	sill,vo%	and,vo%						
min	0.194382E-002	0.285580E-002	0.358730E-003	0.600860E-002	0.822291E-003	7.41739	0.251266E-002	0.655698E-002
	0.986910E-003	0.324544E-001	0.170446E-001					

max 15.0264 42.3855 2.40215 27.4511 65.4408 57.8215 59.8452 26.2887
25.9217 29.7521 30.2444

Output has been written to the 2d tab format file: ex9_1.tab

2d tab format files can be processed with:

PSTABLE - a Perple_X plotting program
PERPLE_X_PLOT - a MATLAB plotting script
PYWERAMI - github.com/ondrolexa/pywerami
spread-sheet programs, e.g., EXCEL

for details on tab format refer to:

perplex.ethz.ch/perplex/faq/Perple_X_tab_file_format.txt

Select operational mode:

- 1 - properties at specified conditions
- 2 - properties on a 2d grid
- 3 - properties along a 1d path
- 4 - as in 3, but input from file
- 0 - EXIT

0

At the end, you have a new file (ex9_1.tab) in the Perple_X folder.

(6) Calculating ISOPLETHS (WERAMI)

This section explains how to calculate COMPOSITIONAL ISOPLETHS for specific phases.

In this example, the XMg (Mg/Mg+Fe) for chlorite, staurolite, garnet and biotite is calculated.

C:\PERPLEX\Perplex691>werami

Perple_X version 6.9.1, source updated January 14, 2022.

Copyright (C) 1986-2022 James A D Connolly <www.perplex.ethz.ch/copyright.html>.

Enter the project name (the name assigned in BUILD) [default = my_project]:

ex9

Reading Perple_X options from: perplex_option.dat

Writing Perple_X option summary to: not requested

Perple_X computational option settings for WERAMI:

Keyword: Value: Permitted values [default]:

Input/Output options:

aqueous_output T [F] T

aqueous_species 20 [20] 0-150

aq_solvent_composition y [y] m: y => mol fraction, m => molality

aq_solute_composition m y [m]: y => mol fraction, m => molality

spreadsheet T [F] T

logarithmic_p F [F] T

bad_number NaN [NaN]

composition_constant F [F] T

composition_phase mol [mol] wt
 composition_system wt [wt] mol
 proportions vol [vol] wt mol
 absolute F [F] T
 cumulative F [F] T
 fancy_cumulative_modes F [F] T
 interpolation on [on] off
 melt_is_fluid F [F] T
 solution_names mod [model] abbreviation full
 structural_formulae T [T] F
 output_species T [T] F
 output_species_props F [F] T
 seismic_output som [some] none all
 pause_on_error T [T] F
 poisson_test F [F] T
 interim_results aut [auto] off manual
 sample_on_grid T [T] F
 auto_exclude T [T] F

Information file output options:

option_list_files F [F] T; echo computational options

Thermodynamic options:

approx_alpha T [T] F
 Anderson-Gruneisen F [F] T
 hybrid_EoS_H2O 4 [4] 0-2, 4-7
 hybrid_EoS_CO2 4 [4] 0-4, 7
 hybrid_EoS_CH4 0 [0] 0-1, 7
 fd_expansion_factor 2.0 [2] >0
 finite_difference_p 0.1E+05 [1d4] >0; fraction = 0.1E-02 [1d-2]

Seismic wavespeed computational options:

seismic_data_file T [F] T
 bounds VRH [VRH] HS
 vrh/hs_weighting 0.5 [0.5] 0->1
 explicit_bulk_modulus T [T] F
 poisson_ratio on [on] all off; Poisson ratio = 0.35
 seismic_output som [some] none all
 poisson_test F [F] T
 Tisza_test F [F] T

To change these options see: www.perplex.ethz.ch/perplex_options.html

 Select operational mode:

- 1 - properties at specified conditions
- 2 - properties on a 2d grid
- 3 - properties along a 1d path
- 4 - as in 3, but input from file
- 0 - EXIT

2

Select a property:

- 1 - Specific Enthalpy (J/m³)
- 2 - Density (kg/m³)

- 3 - Specific heat capacity (J/K/m³)
- 4 - Expansivity (1/K, for volume)
- 5 - Compressibility (1/bar, for volume)
- 6 - Composition (Mol, Mass, or Wt%) of the system
- 7 - Mode (Vol, Mol, or Wt proportion) of a phase
- 8 - Composition (Mol, Mass, or Wt%) of a solution phase
- 9 - Grueneisen thermal ratio
- 10 - Adiabatic bulk modulus (bar)
- 11 - Adiabatic shear modulus (bar)
- 12 - Sound velocity (km/s)
- 13 - P-wave velocity (V_p, km/s)
- 14 - S-wave velocity (V_s, km/s)
- 15 - V_p/V_s
- 16 - Specific entropy (J/K/m³)
- 17 - Entropy (J/K/kg)
- 18 - Enthalpy (J/kg)
- 19 - Heat Capacity (J/K/kg)
- 20 - Specific mass of a phase (kg/m³-system)
- 21 - Poisson ratio
- 22 - Molar Volume (J/bar)
- 23 - Dependent potentials (J/mol, bar, K)
- 24 - Assemblage Index
- 25 - Modes of all phases
- 26 - Sound velocity T derivative (km/s/K)
- 27 - P-wave velocity T derivative (km/s/K)
- 28 - S-wave velocity T derivative (km/s/K)
- 29 - Adiabatic bulk modulus T derivative (bar/K)
- 30 - Shear modulus T derivative (bar/K)
- 31 - Sound velocity P derivative (km/s/bar)
- 32 - P-wave velocity P derivative (km/s/bar)
- 33 - S-wave velocity P derivative (km/s/bar)
- 34 - Adiabatic bulk modulus P derivative (unitless)
- 35 - Shear modulus P derivative (unitless)
- 36 - All phase &/or system properties
- 37 - Absolute amount (Vol, Mol, or Wt) of a phase
- 38 - Multiple property output
- 39 - Heat capacity ratio (C_p/C_v)
- 40 - Lagged or back-calculated aqueous solute chemistry

8

Enter solution (left justified):

Gt(W)

Define the composition in terms of the species/endmembers of Gt(W) (y/n)?

Answer no to define a composition in terms of the systems components.

Answer NO to define a composition in terms of the systems components (e.g. MgO, FeO, etc.)

Answer YES to define a composition in terms of the solid solution end-members (e.g. Prp, Alm, etc.)

Units (mass or molar) are controlled by the composition keyword in perplex_option.dat.

Phase compositions can be computed as mol% or wt%. The default value is mol%. You can control this parameter modifying the "composition_phase" keyword in the perplex_option.dat file

n

Compositions are defined as a ratio of the form:

$$\text{Sum } \{w(i)*n(i), i = 1, c1\} / \text{Sum } \{w(i)*n(i), i = c2, c3\}$$

n(j) = molar amount of component j

w(j) = weighting factor of component j (usually 1)

How many components in the numerator of the composition (<15)?

We want to calculate the ratio Mg/(Mg+Fe), this means that we have one component in the numerator (MgO) and two components in the denominator (MgO + FeO)

1

Enter component indices and weighting factors for the numerator:

1 - MgO

2 - Al2O3

3 - K2O

4 - FeO

5 - SiO2

6 - H2O

The WEIGHTING FACTOR corresponds to the number of cations in each component (e.g. for MgO the weighting factor is 1; for K2O the weighting factor is 2 etc.)

1 | index for MgO

1 | weighting factor for MgO

How many components in the denominator of the composition (<14)?

Enter zero to use the numerator as a composition.

2

Enter component indices and weighting factors for the denominator:

1 - MgO

2 - Al2O3

3 - K2O

4 - FeO

5 - SiO2

6 - H2O

1 | index for MgO

1 | weighting factor for MgO

4 | index for FeO

1 | weighting factor for FeO

The compositional variable is:

1.0 MgO

divided by

1.0 MgO + 1.0 FeO

Change it (y/n)?

n

This composition will be designated: C[Gt(W)1]

Select an additional property or enter 0 to finish:

8

Enter solution (left justified):

Chl(W)

Define the composition in terms of the species/endmembers of Chl(W) (y/n)?

Answer no to define a composition in terms of the systems components.

Units (mass or molar) are controlled by the composition keyword in perplex_option.dat.

n

Compositions are defined as a ratio of the form:

$$\text{Sum } \{w(i)*n(i), i = 1, c1\} / \text{Sum } \{w(i)*n(i), i = c2, c3\}$$

n(j) = molar amount of component j

w(j) = weighting factor of component j (usually 1)

How many components in the numerator of the composition (<15)?

1

Enter component indices and weighting factors for the numerator:

1 - MgO

2 - Al2O3

3 - K2O

4 - FeO

5 - SiO2

6 - H2O

1

1

How many components in the denominator of the composition (<14)?

Enter zero to use the numerator as a composition.

2

Enter component indices and weighting factors for the denominator:

1 - MgO

2 - Al2O3

3 - K2O

4 - FeO

5 - SiO2

6 - H2O

1

1

4

1

The compositional variable is:

1.0 MgO

divided by

1.0 MgO + 1.0 FeO

Change it (y/n)?

n

This composition will be designated: C[Chl(W)2]

Select an additional property or enter 0 to finish:

8

Enter solution (left justified):

St(W)

Define the composition in terms of the species/endmembers of St(W) (y/n)?

Answer no to define a composition in terms of the systems components.

Units (mass or molar) are controlled by the composition keyword in perplex_option.dat.

n

Compositions are defined as a ratio of the form:

$$\text{Sum } \{w(i)*n(i), i = 1, c1\} / \text{Sum } \{w(i)*n(i), i = c2, c3\}$$

n(j) = molar amount of component j

w(j) = weighting factor of component j (usually 1)

How many components in the numerator of the composition (<15)?

1

Enter component indices and weighting factors for the numerator:

1 - MgO

2 - Al2O3

3 - K2O

4 - FeO

5 - SiO2

6 - H2O

1

1

How many components in the denominator of the composition (<14)?

Enter zero to use the numerator as a composition.

2

Enter component indices and weighting factors for the denominator:

1 - MgO

2 - Al2O3

3 - K2O

4 - FeO

5 - SiO2

6 - H2O

1
1
4
1

The compositional variable is:

1.0 MgO

divided by

1.0 MgO + 1.0 FeO

Change it (y/n)?

n

This composition will be designated: C[St(W)3]

Select an additional property or enter 0 to finish:

8

Enter solution (left justified):

Bi(W)

Define the composition in terms of the species/endmembers of Bi(W) (y/n)?

Answer no to define a composition in terms of the systems components.

Units (mass or molar) are controlled by the composition keyword inperplex_option.dat.

n

Compositions are defined as a ratio of the form:

$$\text{Sum } \{w(i)*n(i), i = 1, c1\} / \text{Sum } \{w(i)*n(i), i = c2, c3\}$$

n(j) = molar amount of component j

w(j) = weighting factor of component j (usually 1)

How many components in the numerator of the composition (<15)?

1

Enter component indices and weighting factors for the numerator:

1 - MgO

2 - Al2O3

3 - K2O

4 - FeO

5 - SiO2

6 - H2O

1

1

How many components in the denominator of the composition (<14)?

Enter zero to use the numerator as a composition.

2

Enter component indices and weighting factors for the denominator:

- 1 - MgO
- 2 - Al2O3
- 3 - K2O
- 4 - FeO
- 5 - SiO2
- 6 - H2O

1
1
4
1

The compositional variable is:

1.0 MgO
divided by
1.0 MgO + 1.0 FeO
Change it (y/n)?

n

This composition will be designated: C[Bi(W)4]

Select an additional property or enter 0 to finish:

0

Change default variable range (y/n)?

n

Select the grid resolution (to use an arbitrary grid set sample_on_grid to F):

- 1 - 60 x 60 nodes
- 2 - 119 x 119 nodes
- 3 - 237 x 237 nodes
- 4 - 473 x 473 nodes [default]

4

...

...

Data ranges excluding values equal to bad_number (NaN) specified in perplex_option.dat:

	C[Gt(W)1]	C[Chl(W)2]	C[St(W)3]	C[Bi(W)4]
min	0.117825	0.471855	0.144985	0.313191
max	0.267632	0.638718	0.339163	0.584906

Output has been written to the 2d tab format file: ex9_2.tab

2d tab format files can be processed with:

- PSTABLE - a Perple_X plotting program
- PERPLE_X_PLOT - a MATLAB plotting script
- PYWERAMI - github.com/ondrolexa/pywerami
- spread-sheet programs, e.g., EXCEL

for details on tab format refer to:

perplex.ethz.ch/perplex/faq/Perple_X_tab_file_format.txt

Select operational mode:

- 1 - properties at specified conditions
- 2 - properties on a 2d grid
- 3 - properties along a 1d path
- 4 - as in 3, but input from file
- 0 - EXIT

0

At the end, you have a new file (ex9_2.tab) in the Perple_X folder.

(7) Plotting isomodes and compositional isopleths (PYWERAMI)

Use PYWERAMI to plot the calculated isomodes and compositional isopleths.

You can download Pywerami at this link from the Perple_X website (PyWerami - a free alternative to MatLab): <https://petrol.natur.cuni.cz/~ondro/oldweb/pywerami:home>
Install Pywerami on your pc.

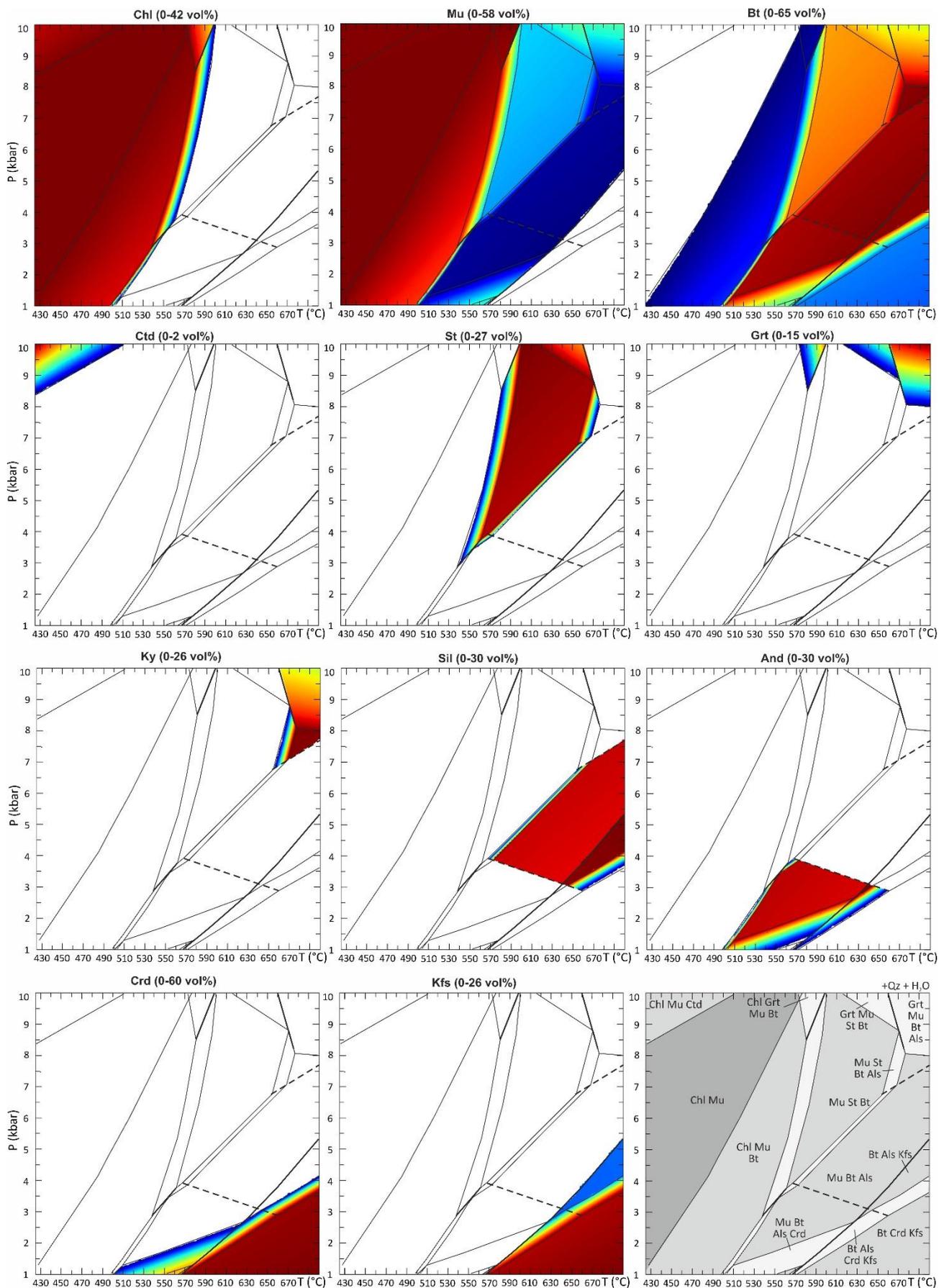
Run PYWERAMI to plot isopleths and isomodes.

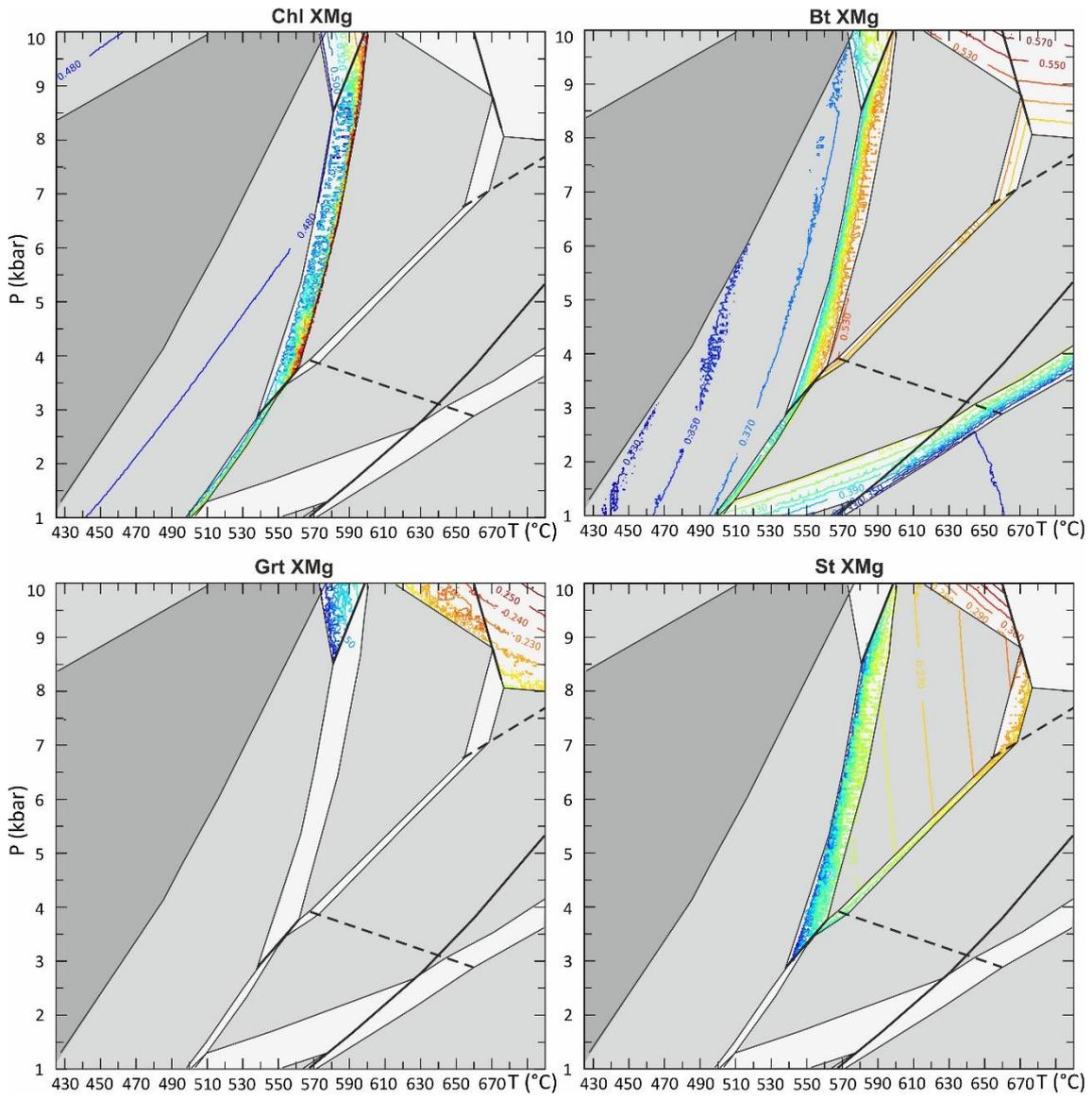
From Pywerami, open the .tab file.

Use the drop-down menu on the right to select the property you want to plot (e.g. Gt(W)vo%)

You can modify the minimum and maximum values to be plotted, as well as the interval between the isopleths/isomodes.

You can save the image in .jpg or (**BETTER IF YOU WANT TO MODIFY THE FIGURE**) in .ps or .svg.





Ex 10

Ex.10 – P-T pseudosection for a METAPELITE in the MnNKCfMASH system

This exercise is intended to explore the influence of some minor components (Na₂O, CaO and MnO) on the topology of the pseudosection calculated for the metapelite sample investigated in Ex. 9. The exercise also explains how to calculate CUMULATIVE MODES along a geothermal gradient.

This exercise is based on the paper by Tinkham et al. (2001) [Geol. Mat. Res., 3, 1-42]. The modelled sample is AWBZ (see Table 1 and their Fig. 5a).

Total bulk composition (mol%; SiO₂ in excess):

Al₂O₃=37.99, FeO=21.93, MgO=19.59, MnO=0.42, CaO=4.95, Na₂O=6.11, K₂O=9.01

T=425-700°C

P=1-10 kbar

(1) Definition of the problem (BUILD)

Because the problem is the same as in Ex. 9, except for the addition of Na₂O, CaO and MnO components **you can edit the ex9.dat input file** (remember to re-name the file as Ex10). Thus, the thermodynamic components are:

```
begin thermodynamic component list
Na2O 1 6.11000 0.00000 0.00000 molar amount
MgO 1 19.5900 0.00000 0.00000 molar amount
Al2O3 1 37.9900 0.00000 0.00000 molar amount
K2O 1 9.01000 0.00000 0.00000 molar amount
CaO 1 4.95000 0.00000 0.00000 molar amount
MnO 1 0.42000 0.00000 0.00000 molar amount
FeO 1 21.9300 0.00000 0.00000 molar amount
end thermodynamic component list
```

Adding Na₂O and CaO additionally implies that the ternary feldspar (plagioclase + K-feldspar) and the white mica (muscovite + paragonite) solid solution models should be added to the calculation.

```
begin solution phase list
Chl (W)
Bi (W)
Mica (W)
Gt (W)
Ctd (W)
St (W)
Crd (W)
feldspar
end solution phase list
```

(2) Doing the calculation (VERTEX)

Run VERTEX to make the calculation:

C:\PERPLEX\Perplex691>vertex

Perple_X version 6.9.1, source updated January 14, 2022.

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Enter the project name (the name assigned in BUILD) [default = my_project]:

ex10

...

(3) Plotting the calculated phase diagram (PSSECT)

Run PSSECT to plot the calculated pseudosection:

```
C:\PERPLEX\Perplex691>pssect
```

Perple_X version 6.9.1, source updated January 14, 2022.

Copyright (C) 1986-2022 James A D Connolly <www.perplex.ethz.ch/copyright.html>.

Enter the project name (the name assigned in BUILD) [default = my_project]:

ex10

Reading Perple_X options from: perplex_option.dat

Perple_X plot options are currently set as:

Keyword:	Value:	Permitted values [default]:
axis_label_scale	1.20	[1.2] (rel)
bounding_box :		
	0	[0] x-min (pts)
	0	[0] y-min (pts)
	800	[800] x-length (pts)
	800	[800] y-length (pts)
field_fill	T	[T] F
field_label	T	[T] F
numeric_field_label	F	[F] T, if T PSSECT writes list to *_assemblages.txt
replicate_label	0.250	0->1 [0.025]
field_label_scale	0.75	[0.72] (rel)
font	Helvetica	
grid	F	[F] T
half_ticks	T	[T] F
line_width	1.00	0-99 [1.] (pts)
picture_transformation :		
	0.180	[0.18] x-scale (rel)
	0.180	[0.18] y-scale (rel)
	130.	[0.18] x-translation (pts)
	220.	[0.18] y-translation (pts)
	0.00	[0.0] rotation (deg)
plot_aspect_ratio	1.000	[1.0] x_axis_length/y_axis_length
splines	T	[T] F
tenth_ticks	F	[F] T
text_scale	1.000	[1.] (rel)
plot_extra_data		

To change these options edit or create the plot option file

See: www.perplex.ethz.ch/perplex_plot_options.html

PostScript will be written to file: ex10.ps

Modify the default plot (y/n)?

n

There are 10 fields for: Mica(W) feldspar Bi(W) Chl(W) zo ab

There are 7 fields for: feldspar Chl(W) Gt(W) Mica(W) Bi(W) zo ab

There are 3 fields for: Crd(W) Bi(W) feldspar feldspar Mica(W)

There are 10 fields for: St(W) feldspar Mica(W) Bi(W) Gt(W) sill

..

In the resulting diagram, both plagioclase and K-feldspar are reported as “feldspar”. Thus, fields containing two feldspars contain both plagioclase and K-feldspar, whereas those containing one feldspar can contain either plagioclase or K-feldspar. **To know which of the two feldspars is stable in a given field, use WERAMI option 1 (properties at specified conditions), e.g. at 753 K, 3000 bar:**

Stable phases at:

T(K) = 753.000
P(bar) = 3000.00
Y(CO2) = 0.00000

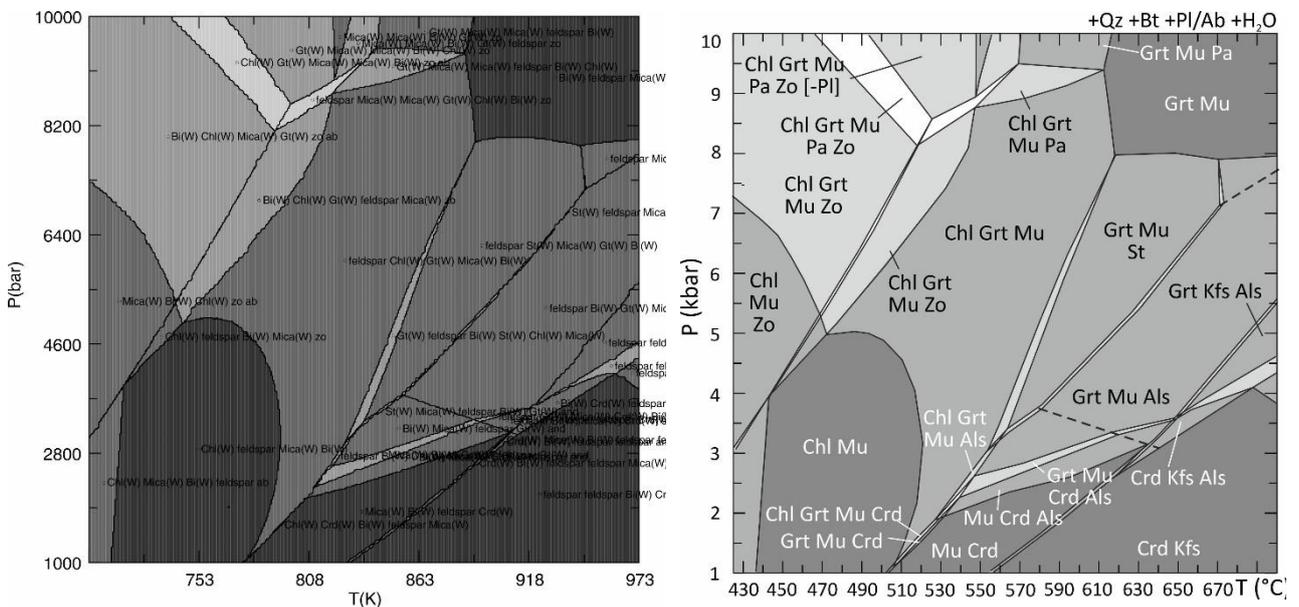
Phase Compositions (molar proportions):

	wt %	vol %	mol %	mol	Na2O	MgO	Al2O3	K2O	CaO	MnO	FeO	SiO2	H2O
Chl(W)	17.78	17.21	10.92	4.31	0.00000	2.56888	1.22106	0.00000	0.00000	0.05786	2.15220	2.77894	4.00000
feldspar	27.64	29.69	39.72	15.7	0.34063	0.00000	0.65666	0.00271	0.31332	0.00000	0.00000	2.68668	0.00000
Mica(W)	32.05	32.30	31.02	12.3	0.06244	0.03159	1.44627	0.43620	0.00273	0.00000	0.02351	3.05236	1.00000
Bi(W)	22.53	20.80	18.34	7.25	0.00000	1.12162	0.64861	0.50000	0.00000	0.02354	1.70624	2.85139	1.00000

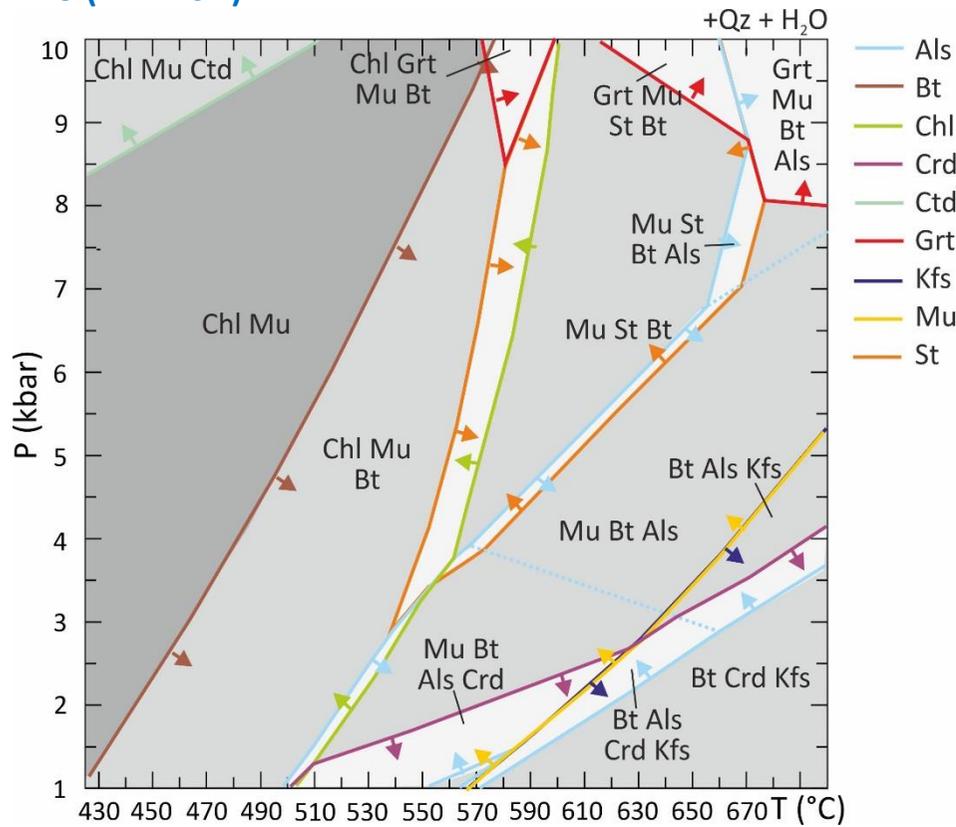
Phase speciation (molar proportions):

Chl(W) mnchl: 0.01157, daph: 0.46915, ames: 0.22111, afchl: 0.19367, clin: 0.29812, och1: 0.00002, och2: -0.19364
feldspar abh: 0.68125, an: 0.31332, san: 0.00542
Mica(W) mu: 0.81729, pa: 0.12487, ma1_dqf: 0.00273, cel: 0.03159, fcel: 0.02351
Bi(W) mnbi: 0.00785, east: 0.14861, ann: 0.55021, phi: 0.23772, obi: 0.05562

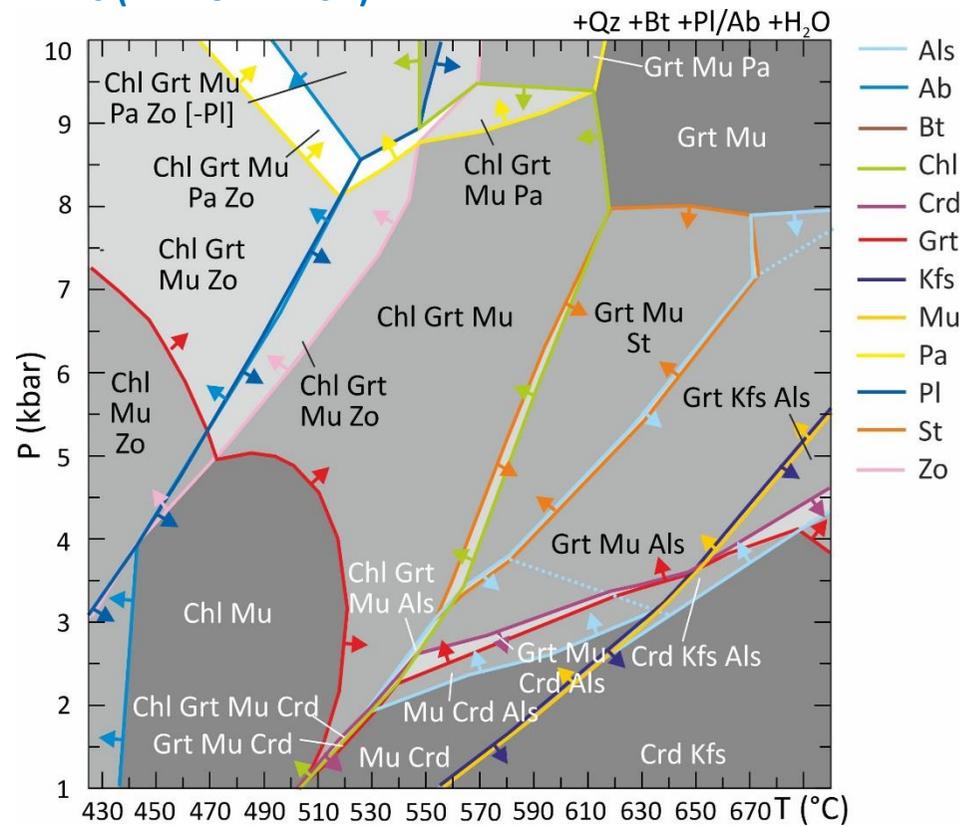
The feldspar stable at 753 K, 3000 bar is a plagioclase.



Ex.9 (KFMASH)



Ex. 10 (MnNCKFMASH)

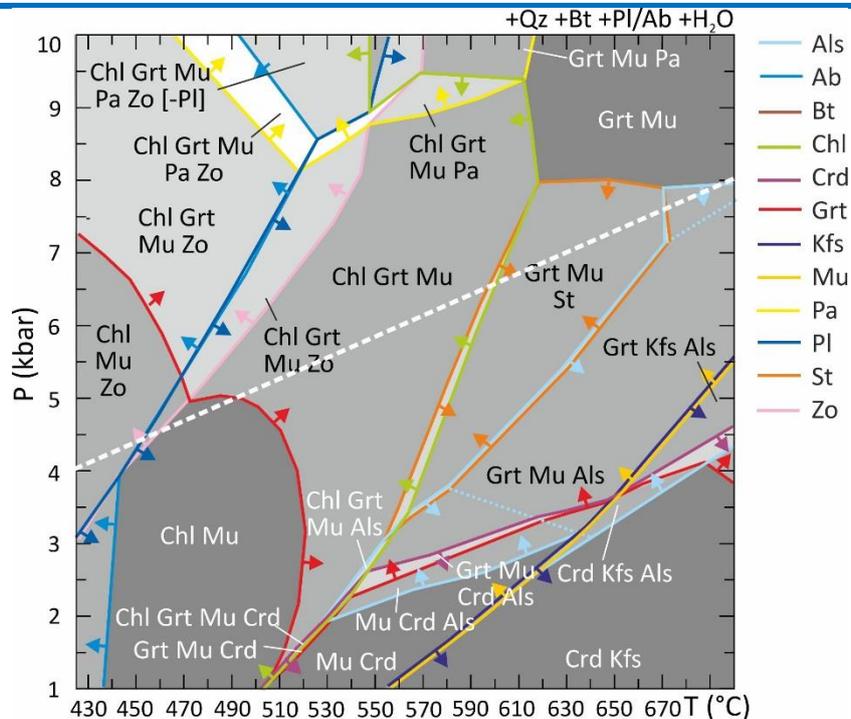


Comparing this pseudosection with that modelled in Ex. 9 (KFMASH system), it appears that the introduction of Na₂O, CaO and MnO has the following consequences:

- The garnet stability field is significantly enlarged toward low P and T with respect to the pseudosection of Ex. 9;
- Chloritoid is no more stable;
- The biotite stability field is significantly enlarged toward lower T (biotite is predicted to be stable in all the fields);
- Plagioclase and/or albite is predicted to be stable in most of the fields;
- Zoisite appears at low T.

(4) Calculating cumulative modes along a geothermal gradient (WERAMI)

This section explains how to calculate the **variation in the modal amounts** of all the phase (vol%) along a geothermal gradient defined as: $P \text{ (bar)} = 15 T \text{ (K)} - 6545$ (corresponding to the white dashed line reported in the pseudosection below).



Use an excel spreadsheet to create the input file for the definition of the P/T gradient. The input file should consist of two columns only, i.e. the first column contains the temperatures (in Kelvin), the second column contains the pressures (in bar). Consider the temperatures range 430-700°C (703-973 K), and temperature values with an interval of 1°C; derive pressure values according to the equation $P \text{ (bar)} = 15 T \text{ (K)} - 6545$. Save the file as a .txt file named “grad.txt”,

Run WERAMI to calculate the MODES of ALL the phases.

```
C:\PERPLEX\Perplex691>werami
```

Perple_X version 6.9.1, source updated January 14, 2022.

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Enter the project name (the name assigned in BUILD) [default = my_project]:

ex10

Reading Perple_X options from: perple_x_option.dat

Writing Perple_X option summary to: not requested

Perple_X computational option settings for WERAMI:

Keyword: Value: Permitted values [default]:

Input/Output options:

aqueous_output T [F] T
 aqueous_species 20 [20] 0-150
 aq_solvent_composition y [y] m: y => mol fraction, m => molality
 aq_solute_composition m y [m]: y => mol fraction, m => molality
 spreadsheet T [F] T
 logarithmic_p F [F] T
 bad_number NaN [NaN]
 composition_constant F [F] T
 composition_phase mol [mol] wt
 composition_system wt [wt] mol
 proportions vol [vol] wt mol
 absolute F [F] T
 cumulative F [F] T
 fancy_cumulative_modes F [F] T
 interpolation on [on] off
 melt_is_fluid F [F] T
 solution_names mod [model] abbreviation full
 structural_formulae T [T] F
 output_species T [T] F
 output_species_props F [F] T
 seismic_output som [some] none all
 pause_on_error T [T] F
 poisson_test F [F] T
 interim_results aut [auto] off manual
 sample_on_grid T [T] F
 auto_exclude T [T] F

Information file output options:

option_list_files F [F] T; echo computational options

Thermodynamic options:

approx_alpha T [T] F
 Anderson-Gruneisen F [F] T
 hybrid_EoS_H2O 4 [4] 0-2, 4-7
 hybrid_EoS_CO2 4 [4] 0-4, 7
 hybrid_EoS_CH4 0 [0] 0-1, 7
 fd_expansion_factor 2.0 [2] >0
 finite_difference_p 0.1E+05 [1d4] >0; fraction = 0.1E-02 [1d-2]

Seismic wavespeed computational options:

seismic_data_file T [F] T
 bounds VRH [VRH] HS
 vrh/hs_weighting 0.5 [0.5] 0->1
 explicit_bulk_modulus T [T] F
 poisson_ratio on [on] all off; Poisson ratio = 0.35
 seismic_output som [some] none all
 poisson_test F [F] T
 Tisza_test F [F] T

To change these options see: www.perplex.ethz.ch/perplex_options.html

Select operational mode:

- 1 - properties at specified conditions
- 2 - properties on a 2d grid

- 3 - properties along a 1d path
- 4 - as in 3, but input from file
- 0 - EXIT

4

Select option 4 if you would like to use the geothermal gradient as defined in the grad.txt file.

Path will be described by:

- 1 - a file containing a polynomial function
- 2 - a file containing a list of x-y points

Enter 1 or 2:

2

Enter the file name:

grad.txt

File contains 271 points

every nth plot will be plotted, enter n:

1

Here you can specify if you want to use all the P-T points defined in the input file, or if you want to use a different P(T) interval. Answering 1 means that you want to use all the points as defined in the input file.

Select a property:

- 1 - Specific Enthalpy (J/m³)
- 2 - Density (kg/m³)
- 3 - Specific heat capacity (J/K/m³)
- 4 - Expansivity (1/K, for volume)
- 5 - Compressibility (1/bar, for volume)
- 6 - Composition (Mol, Mass, or Wt%) of the system
- 7 - Mode (Vol, Mol, or Wt proportion) of a phase
- 8 - Composition (Mol, Mass, or Wt%) of a solution phase
- 9 - Grueneisen thermal ratio
- 10 - Adiabatic bulk modulus (bar)
- 11 - Adiabatic shear modulus (bar)
- 12 - Sound velocity (km/s)
- 13 - P-wave velocity (V_p, km/s)
- 14 - S-wave velocity (V_s, km/s)
- 15 - V_p/V_s
- 16 - Specific entropy (J/K/m³)
- 17 - Entropy (J/K/kg)
- 18 - Enthalpy (J/kg)
- 19 - Heat Capacity (J/K/kg)
- 20 - Specific mass of a phase (kg/m³-system)
- 21 - Poisson ratio
- 22 - Molar Volume (J/bar)
- 23 - Dependent potentials (J/mol, bar, K)
- 24 - Assemblage Index
- 25 - Modes of all phases
- 26 - Sound velocity T derivative (km/s/K)
- 27 - P-wave velocity T derivative (km/s/K)
- 28 - S-wave velocity T derivative (km/s/K)

- 29 - Adiabatic bulk modulus T derivative (bar/K)
- 30 - Shear modulus T derivative (bar/K)
- 31 - Sound velocity P derivative (km/s/bar)
- 32 - P-wave velocity P derivative (km/s/bar)
- 33 - S-wave velocity P derivative (km/s/bar)
- 34 - Adiabatic bulk modulus P derivative (unitless)
- 35 - Shear modulus P derivative (unitless)
- 36 - All phase &/or system properties
- 37 - Absolute amount (Vol, Mol, or Wt) of a phase
- 38 - Multiple property output
- 39 - Heat capacity ratio (Cp/Cv)
- 40 - Lagged or back-calculated aqueous solute chemistry

25

Option 25 allows to simultaneously calculate the mode of all the phases.

Output cumulative modes (y/n)?

(see www.perplex.ethz.ch/perplex_options.html#cumulative_modes)

n

Although our aim is to calculate CUMULATIVE MODES, I suggest to not select the “cumulative mode” option here, because it is more easy to plot “normal” modes (i.e. not cumulative) using EXCEL rather than the “cumulative” modes using PSSECT.

Include fluid in computation of aggregate (or modal) properties (y/n)?

n

warning ver178 at T(K)= 703.0 P(bar)= 4000.

the shear modulus of: Mica(W)

is missing or invalid and has been estimated from the default poisson ratio

...

...

Data ranges excluding values equal to bad_number (NaN) specified in perplex_option.dat:

	Chl(W)	Mica(W)	Mica(W)	Bi(W)	feldspar	feldspar	ab	zo	Gt(W)	Crd(W)
and	St(W)	sill	ky							
min	2.58924	21.2616	0.100000E+100	13.2468	27.9172	0.100000E+100	20.1750	0.930910E-001		
	0.281598E-001	0.100000E+100	0.100000E+100	0.951214	0.100000E+100	0.264885E-002				
max	21.5547	38.3932	-0.100000E+100	37.0166	31.3358	-0.100000E+100	20.5347	6.29074		
	14.8779	-0.100000E+100	-0.100000E+100	5.73130	-0.100000E+100	0.768047				

Output has been written to two files:

plt format is in file: ex10_1.plt

1d tab format is in file: ex10_1.tab

plt format files can be plotted with:

PSVDRAW

1d tab format files can be processed with:

PSTABLE - a Perple_X plotting program

PERPLE_X_PLOT - a Matlab plotting script

spread-sheet programs, e.g., EXCEL

for details on tab format refer to:

perplex.ethz.ch/perplex/faq/Perple_X_tab_file_format.txt

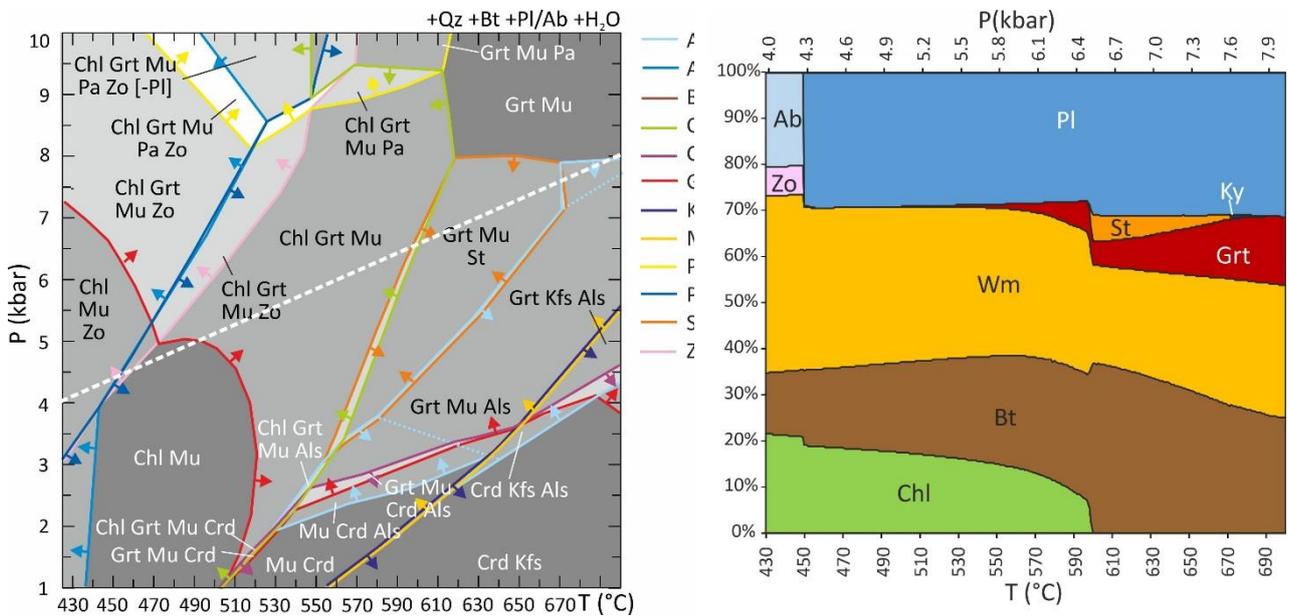
Select operational mode:

- 1 - properties at specified conditions
- 2 - properties on a 2d grid
- 3 - properties along a 1d path
- 4 - as in 3, but input from file
- 0 - EXIT

0

At the end, you have a new file (ex10_1.tab) in the Perple_X folder.

You can open the ex10_1.tab file using EXCEL; replace the NaN values with 0 and plot the data using the option Area Graph.



Ex 11

Ex. 11 – T-XMg pseudosection for a METAPELITE in the MnNKCFMASH system

This exercise is intended to explore the influence of bulk XMg [$\text{MgO}/(\text{MgO}+\text{FeO})$] on the stability field of the main mineral assemblages, for the same metapelite sample investigated in Ex. 9 and 10.

The exercise provides the opportunity to calculate an isobaric T-X pseudosection (i.e. a phase diagram section with a compositional parameter on the horizontal axis).

This exercise is based on the paper by Tinkham et al. (2001) [Geol. Mat. Res., 3, 1-42]. The modelled sample is AWBZ (see Table 1 and their Fig. 10).

The T-XMg pseudosection is calculated at a fixed pressure of 3.5 kbar and for XMg ranging between 0 and 1. The XMg of the metapelite investigated in Ex. 10 is $\text{XMg}=0.47$.

The two bulk compositions to be used are (mol%; SiO₂ in excess):

XMg=0: Al₂O₃=37.99, FeO=41.52, MgO=0.00, MnO=0.42, CaO=4.95, Na₂O=6.11, K₂O=9.01

XMg=1: Al₂O₃=37.99, FeO=0.00, MgO=41.52, MnO=0.42, CaO=4.95, Na₂O=6.11, K₂O=9.01

T=425-700°C

P=3.5 kbar

Use the same solid solution models used in Ex. 10

In the perplex_option file, change the solution_names keyword in “abb”, in order to show – in the output - the abbreviation name (rather than the whole model name) for solution models .

(1) Definition of the problem (BUILD)

```
C:\PERPLEX\Perplex691>build
```

Perple_X version 6.9.1, source updated January 14, 2022.

Copyright (C) 1986-2022 James A D Connolly <www.perplex.ethz.ch/copyright.html>.

NO is the default (blank) answer to all Y/N prompts

Enter a name for this project (the name will be used as the root for all output file names) [default = my_project]:

ex11

The problem definition file will be named: ex11.dat

Enter thermodynamic data file name [default = hp02ver.dat]:

hp62ver.dat

Enter the computational option file name [default = perplex_option.dat]:

See: www.perplex.ethz.ch/perplex_options.html

[enter]

Reading Perple_X options from: perplex_option.dat

The current data base components are:

Na2O MgO Al2O3 SiO2 K2O CaO TiO2 MnO FeO NiO ZrO2 Cl2 O2 H2O CO2 CuO Cr2O3 S2 F2 N2 ZnO

Transform them (Y/N)?

N

Specify computational mode:

- 1 - Convex-Hull minimization
- 2 - Constrained minimization on a 2d grid [default]
- 3 - Constrained minimization on a 1d grid
- 4 - Output pseudocompound data
- 5 - 1-d Phase fractionation
- 6 - 0-d Infiltration-reaction-fractionation
- 7 - 2-d Phase fractionation (FRAC2D and TITRATE reactive transport models)

Use Convex-Hull minimization for Schreinemakers projections or phase diagrams with > 2 independent variables. Use constrained minimization for phase diagrams or phase diagram sections with < 3 independent variables.

2

Calculations with a saturated fluid (Y/N)?

y

Select the independent saturated fluid components:

H2O CO2

Enter names, 1 per line, press <enter> to finish:

For C-O-H fluids it is only necessary to select volatile species present in the solids of interest. If the species listed here are H2O and CO2, then to constrain O2 chemical potential to be consistent with C-O-H fluid speciation treat O2 as a saturated component. Refer to the Perple_X Tutorial for details.

H2O

Calculations with saturated components (Y/N)?

y

****warning ver015**** if you select > 1 saturated component, then the order you enter the components determines the saturation heirarchy and may effect your results (see Connolly 1990).

Select < 6 saturated components from the set:

Na2O MgO Al2O3 SiO2 K2O CaO TiO2 MnO FeO NiO ZrO2 Cl2 O2 CO2 CuO Cr2O3 S2 F2 N2 ZnO

Enter names, 1 per line, press <enter> to finish:

SiO2

Use chemical potentials, activities or fugacities as independent variables (Y/N)?

n

Select thermodynamic components from the set:

Na2O MgO Al2O3 K2O CaO TiO2 MnO FeO NiO ZrO2 Cl2 O2 CO2 CuO Cr2O3 S2 F2 ZnO

Enter names, 1 per line, press <enter> to finish:

Na2O

MgO
Al₂O₃
K₂O
CaO
MnO
FeO

Because the thermodynamic data file identifies: H₂O as special components, you will be prompted next for the EoS to be used for the corresponding components and mixtures thereof. To override this behavior, e.g., to use a generic hybrid fluid EoS, delete the special_component section from the thermodynamic data file header.

NOTE: the EoS choice specified here will override the EoS choice specified by the hybrid_EoS option, to override this behavior delete the special_component section from the the thermodynamic data file header.

Select fluid equation of state:

- 0 - X(CO₂) H₂O-CO₂ Modified Redlich-Kwong (MRK) DeSantis et al 74
- 1 - X(CO₂) H₂O-CO₂ HSMRK Kerrick & Jacobs 81
- 2 - X(CO₂) H₂O-CO₂ MRK hybrid-EoS*
- 5 - X(CO₂) H₂O-CO₂ CORK Holland & Powell 91, 98
- 8 - f(O₂/CO₂) C-buffered COH MRK hybrid-EoS*
- 10 - X(O) C-buffered COH MRK hybrid-EoS Connolly & Cesare 93*
- 12 - X(O)-f(S₂) C-buffered COHS MRK hybrid-EoS Connolly & Cesare 93*
- 13 - X(H₂) H₂O-H₂ MRK hybrid-EoS*
- 14 - X(CO₂) H₂O-CO₂ Pitzer & Sterner 94; Holland & Powell mixing 03
- 15 - X(H₂) H₂O-H₂ low T MRK hybrid-EoS*
- 16 - X(O) H-O MRK hybrid-EoS*
- 17 - X(O)-f(S₂) H-O-S MRK hybrid-EoS*
- 19 - X(O)-X(S) C-buffered COHS MRK hybrid-EoS Connolly & Cesare 93*
- 20 - X(O)-X(C) COHS MRK hybrid-EoS Connolly & Cesare 93*
- 24 - f(O₂/CO₂)-N/C C-buffered COHN MRK hybrid-EoS*
- 25 - X(CO₂)-X(NaCl) H₂O-CO₂-NaCl Aranovich et al 10
- 26 - X(O) O-Si MRK Connolly 16
- 27 - X(O)-X(C) C-O-H MRK hybrid-EoS*

*Hybrid EoS use the following pure species EoS, to change these associations modify the hybrid_EoS keywords in the perplex_option file:

- H₂O - PSEoS Pitzer & Sterner 1994
- CO₂ - PSEoS Pitzer & Sterner 1994
- CH₄ - MRK DeSantis et al 1974

5

The data base has P(bar) and T(K) as default independent potentials.

Make one dependent on the other, e.g., as along a geothermal gradient (y/n)?

n

Select x-axis variable:

- 1 - P(bar)
- 2 - T(K)
- 3 - Y(CO₂)
- 4 - Composition X_C1* (user defined)

*Although only one component is specified for the Y(CO₂) phase, its equation of state permits use of its compositional variable:

*X_C1 can not be selected as the y-axis variable

In this case, the x-axis variable is a composition (XMg)

4

Select y-axis variable:

1 - P(bar)

2 - T(K)

3 - Y(CO2)

4 - Composition X_C2 (user defined)

2

Enter minimum and maximum values, respectively, for: T(K)

698

973

Specify sectioning value for: P(bar)

3500

Specify sectioning value for: Y(CO2)

0

For gridded minimization, grid resolution is determined by the number of levels (grid_levels) and the resolution at the lowest level in the X- and Y-directions (x_nodes and y_nodes) these parameters are currently set for the exploratory and autorefine cycles as follows:

stage grid_levels xnodes ynodes effective resolution

exploratory 1 40 40 40 x 40 nodes

auto-refine 4 60 60 473 x 473 nodes

To change these options edit or create the file perplex_option.dat

See: www.perplex.ethz.ch/perplex_options.html#grid_parameters

All thermodynamic components must be constrained, specify saturated components also (Y/N)?

n

Specify component amounts by mass (Y/N)?

n

The amounts you enter next need not be normalized; regardless of units, they define the molar amount of the system

The bulk composition of the system will be computed as:

$$C = C_0*(1 - X_{C1}) + C_1*X_{C1}$$

where X_C1 varies between 0 and 1, and C0 and C1 are the compositions specified next.

To compute bulk compositions as: $C = C_0 + C_1*X_{C1}$ change the computational option keyword closed_c_space.

Enter the molar amounts of the components:

Na2O MgO Al2O3 K2O CaO MnO FeO

to define the composition C0

This corresponds to $X_{MgO}=0$. To avoid problems with O/D solution models approaching the $X_{MgO}=0$ side, I would suggest to set $MgO=0.001$

6.11
0.001
37.99
9.01
4.95
0.42
41.52

Enter the molar amounts of the components:

Na2O MgO Al2O3 K2O CaO MnO FeO

to define the composition C1

This corresponds to $X_{MgO}=1$. To avoid problems with O/D solution models approaching the $X_{MgO}=1$ side, I would suggest to set $FeO=0.001$

6.11
41.52
37.99
9.01
4.95
0.42
0.001

Output a print file (Y/N)?

y

Exclude pure and/or endmember phases (Y/N)?

n

Include solution models (Y/N)?

y

Enter the solution model file name [default = solution_model.dat]:

Enter solution model file name [default = solution_model.dat] left justified, < 100 characters:

[return]

...

Select models from the following list, enter 1 per line, press <enter> to finish

ternary-feldspar models: feldspar feldspar_B Pl(I1,HP) Fsp(C1)

clinoamphibole models: cAmph_I(G) cAmph(G) Cumm Gl Tr...

...

For details on these models see: www.perplex.ethz.ch/perplex_solution_model_glossary.html or read the commentary in the solution model file.

Chl(W)

Bi(W)

Mica(W)

Gt(W)

Ctd(W)

St(W)
Crd(W)
feldspar

Enter calculation title:

Ex11

(2) Doing the calculation (VERTEX)

Run VERTEX to make the calculation:

```
C:\PERPLEX\Perplex691>vertex
```

Perple_X version 6.9.1, source updated January 14, 2022.

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Enter the project name (the name assigned in BUILD) [default = my_project]:

Ex11

....

(3) Plotting the calculated phase diagram (PSSECT)

Run PSSECT to plot the calculated pseudosection:

```
C:\PERPLEX\Perplex691>pssect
```

Perple_X version 6.9.1, source updated January 14, 2022.

Copyright (C) 1986-2022 James A D Connolly <www.perplex.ethz.ch/copyright.html>.

Enter the project name (the name assigned in BUILD) [default = my_project]:

ex11

Reading Perple_X options from: perplex_option.dat

Perple_X plot options are currently set as:

Keyword:	Value:	Permitted values [default]:
axis_label_scale	1.20	[1.2] (rel)
bounding_box :		
	0	[0] x-min (pts)
	0	[0] y-min (pts)
	800	[800] x-length (pts)
	800	[800] y-length (pts)
field_fill	T	[T] F
field_label	T	[T] F
numeric_field_label	F	[F] T, if T PSSECT writes list to *_assemblages.txt
replicate_label	0.250	0->1 [0.025]
field_label_scale	0.75	[0.72] (rel)
font	Helvetica	
grid	F	[F] T
half_ticks	T	[T] F
line_width	1.00	0-99 [1.] (pts)

picture_transformation :

```

0.180 [0.18] x-scale (rel)
0.180 [0.18] y-scale (rel)
130. [0.18] x-translation (pts)
220. [0.18] y-translation (pts)
0.00 [0.0] rotation (deg)
plot_aspect_ratio 1.000 [1.0] x_axis_length/y_axis_length
splines T [T] F
tenth_ticks F [F] T
text_scale 1.000 [1.] (rel)
plot_extra_data

```

To change these options edit or create the plot option file

See: www.perplex.ethz.ch/perplex_plot_options.html

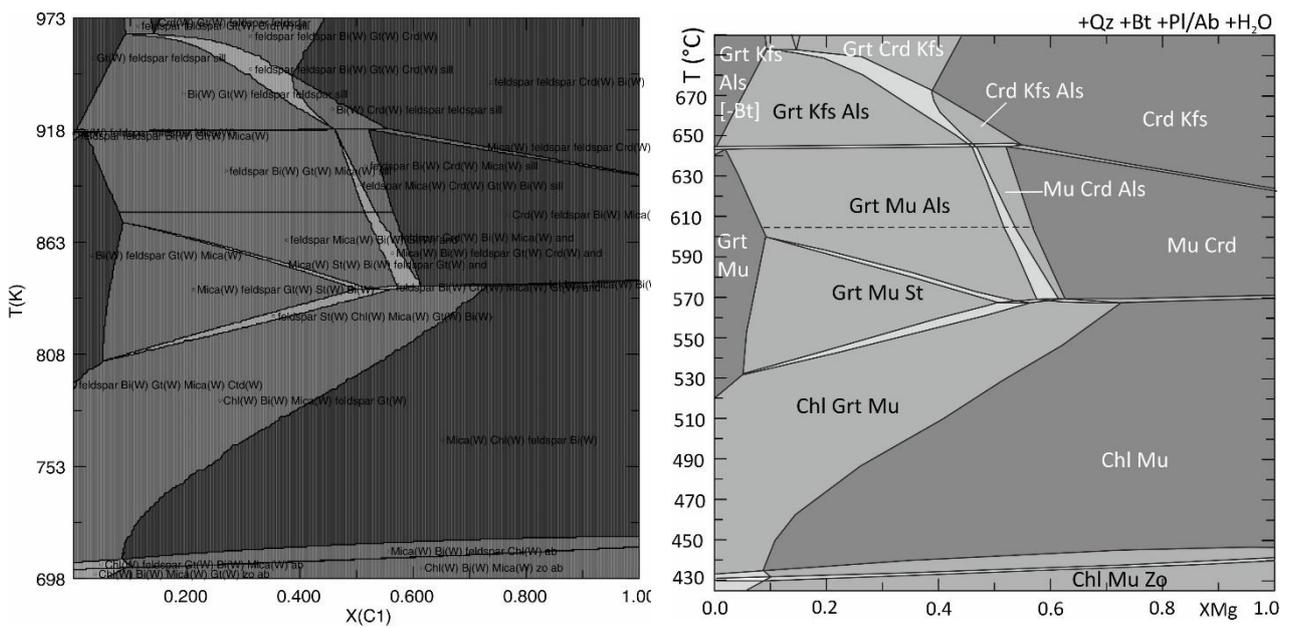
PostScript will be written to file: ex11.ps

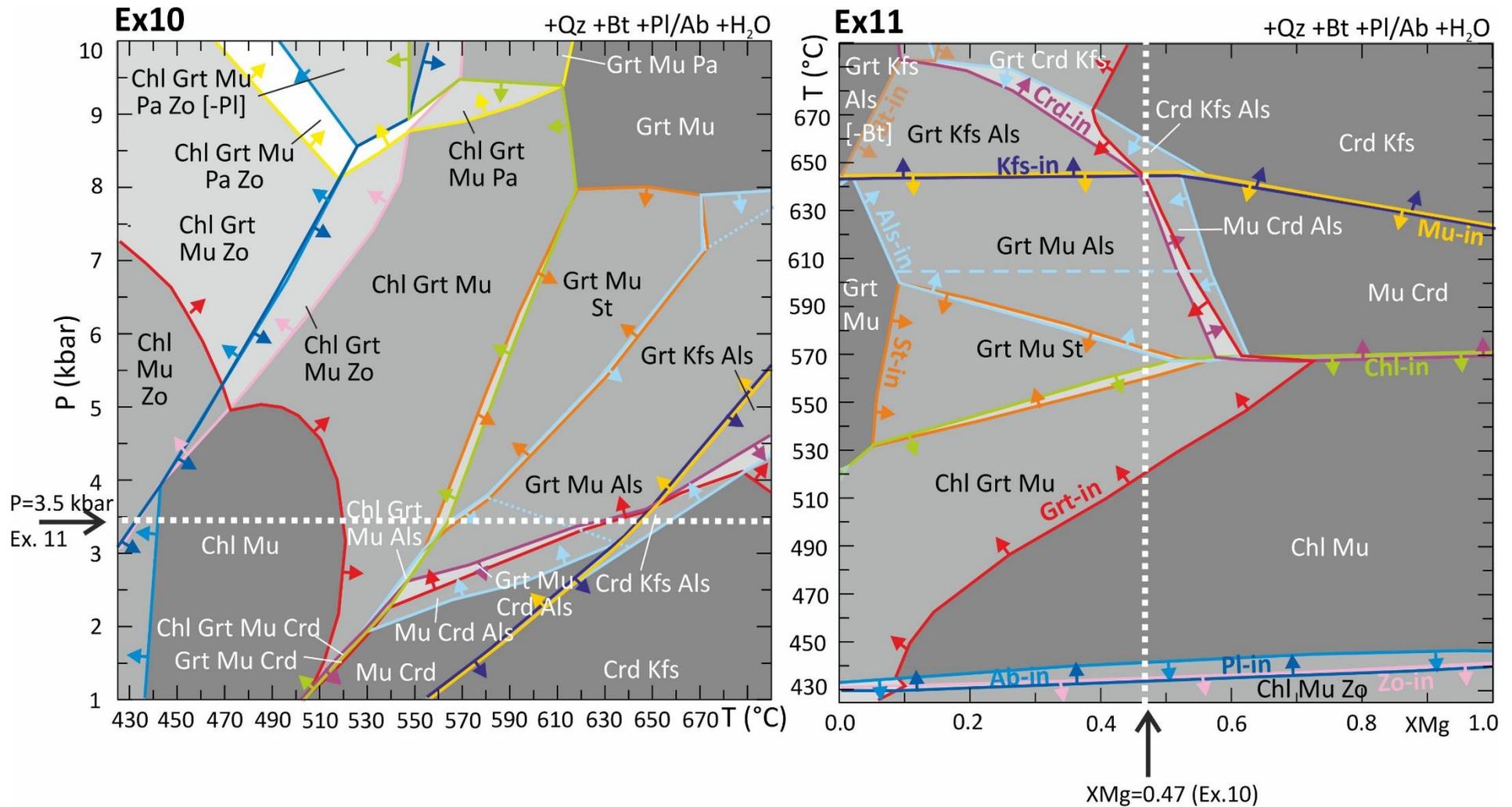
Modify the default plot (y/n)?

n

There are 3 fields for: feldspar feldspar Bi(W) Mica(W) Gt(W) sill

There are 17 fields for: feldspar Mica(W) Bi(W) Chl(W) zo ab





Comparison between the P-T pseudosection calculated in Ex. 10 ($XMgO=0.47$) and the T- $XMgO$ calculated at 3.5 kbar. **The sequence of mineral assemblages at increasing T should correspond in the two pseudosections.**

Ex 12

Ex. 12 – DIRECT modelling of an anatectic METAPELITE (NKCFMASH system)

This exercise deals with the “DIRECT” modelling of a metapelite sample at supra-solidus conditions (i.e. melt-bearing). “Direct modelling” means that you know which is the protolith composition, including its initial H₂O amount (which is generally not the case...). In other words, we will consider a generic metapelite (with an average composition) and we will see what happens to this metapelite if it is heated enough to experience partial melting.

This exercise is based on the paper by White et al. (2001) [J. metam. Geol., 19, 139-153]. The P-T pseudosection is reported in their Fig. 4.

Bulk composition (mol%; SiO₂ in excess):

Al₂O₃=30.66, FeO=23.74, MgO=12.47, CaO=0.97, Na₂O=1.94, K₂O=9.83, H₂O=20.39

T=630-1000°C

P=0-12 kbar

(1) Definition of the problem (BUILD)

```
C:\PERPLEX\Perplex691>build
```

Perple_X version 6.9.1, source updated January 14, 2022.

Copyright (C) 1986-2022 James A D Connolly <www.perplex.ethz.ch/copyright.html>.

NO is the default (blank) answer to all Y/N prompts

Enter a name for this project (the name will be used as the root for all output file names) [default = my_project]:

ex12

The problem definition file will be named: ex12.dat

Enter thermodynamic data file name [default = hp02ver.dat]:

hp62ver.dat

Enter the computational option file name [default = perplex_option.dat]:

See: www.perplex.ethz.ch/perplex_options.html

[enter]

Reading Perple_X options from: perplex_option.dat

The current data base components are:

Na₂O MgO Al₂O₃ SiO₂ K₂O CaO TiO₂ MnO FeO NiO ZrO₂ Cl₂ O₂ H₂O CO₂ CuO Cr₂O₃ S₂ F₂ N₂ ZnO

Transform them (Y/N)?

n

Specify computational mode:

1 - Convex-Hull minimization

- 2 - Constrained minimization on a 2d grid [default]
- 3 - Constrained minimization on a 1d grid
- 4 - Output pseudocompound data
- 5 - 1-d Phase fractionation
- 6 - 0-d Infiltration-reaction-fractionation
- 7 - 2-d Phase fractionation (FRAC2D and TITRATE reactive transport models)

Use Convex-Hull minimization for Schreinemakers projections or phase diagrams with > 2 independent variables. Use constrained minimization for phase diagrams or phase diagram sections with < 3 independent variables.

2

Calculations with a saturated fluid (Y/N)?

Because specification of H₂O as a saturated phase component causes Perple_X to exclude any phases with the H₂O composition that are not named "H₂O", **H₂O should not be specified as a saturated fluid phase in calculations involving a hydrous silicate melt** if, as is commonly the case, the melt model involves a water end-member that is not named "H₂O" (e.g. h₂oL). **This means that, for calculations at supra-solidus conditions (e.g. melt-bearing systems), the user must consider H₂O as a normal chemical component, and not as a saturated fluid phase.**

n

Calculations with saturated components (Y/N)?

y

****warning ver015**** if you select > 1 saturated component, then the order you enter the components determines the saturation heirarchy and may effect your results (see Connolly 1990).

Select < 6 saturated components from the set:

Na₂O MgO Al₂O₃ SiO₂ K₂O CaO TiO₂ MnO FeO NiO ZrO₂ Cl₂ O₂ H₂O CO₂ CuO Cr₂O₃ S₂ F₂

Enter names, 1 per line, press <enter> to finish:

SiO₂

Use chemical potentials, activities or fugacities as independent variables (Y/N)?

n

Select thermodynamic components from the set:

Na₂O MgO Al₂O₃ K₂O CaO TiO₂ MnO FeO NiO ZrO₂ Cl₂ O₂ H₂O CO₂ CuO Cr₂O₃ S₂ F₂ N₂

Enter names, 1 per line, press <enter> to finish:

Na₂O

MgO

Al₂O₃

K₂O

CaO

FeO

H₂O

Because the thermodynamic data file identifies: H₂O as special components, you will be prompted next for the EoS to be used for the corresponding composants and mixtures thereof. To override this behavior, e.g., to use a generic hybrid fluid EoS, delete the special_component section from the thermodynamic data file header.

Select fluid equation of state:

- 0 - X(CO₂) H₂O-CO₂ Modified Redlich-Kwong (MRK) DeSantis et al 74

- 1 - X(CO2) H2O-CO2 HSMRK Kerrick & Jacobs 81
- 2 - X(CO2) H2O-CO2 MRK hybrid-EoS*
- 5 - X(CO2) H2O-CO2 CORK Holland & Powell 91, 98
- 8 - f(O2/CO2) C-buffered COH MRK hybrid-EoS*
- 10 - X(O) C-buffered COH MRK hybrid-EoS Connolly & Cesare 93*
- 12 - X(O)-f(S2) C-buffered COHS MRK hybrid-EoS Connolly & Cesare 93*
- 13 - X(H2) H2O-H2 MRK hybrid-EoS*
- 14 - X(CO2) H2O-CO2 Pitzer & Sterner 94; Holland & Powell mixing 03
- 15 - X(H2) H2O-H2 low T MRK hybrid-EoS*
- 16 - X(O) H-O MRK hybrid-EoS*
- 17 - X(O)-f(S2) H-O-S MRK hybrid-EoS*
- 19 - X(O)-X(S) C-buffered COHS MRK hybrid-EoS Connolly & Cesare 93*
- 20 - X(O)-X(C) COHS MRK hybrid-EoS Connolly & Cesare 93*
- 24 - f(O2/CO2)-N/C C-buffered COHN MRK hybrid-EoS*
- 25 - X(CO2)-X(NaCl) H2O-CO2-NaCl Aranovich et al 10
- 26 - X(O) O-Si MRK Connolly 16
- 27 - X(O)-X(C) C-O-H MRK hybrid-EoS*

*Hybrid EoS use the following pure species EoS, to change these associations modify the hybrid_EoS keywords in the perplex_option file:

- H2O - PSEoS Pitzer & Sterner 1994
- CO2 - PSEoS Pitzer & Sterner 1994
- CH4 - MRK DeSantis et al 1974

5

The data base has P(bar) and T(K) as default independent potentials.
Make one dependent on the other, e.g., as along a geothermal gradient (y/n)?

n

Select x-axis variable:

- 1 - P(bar)
- 2 - T(K)
- 3 - Composition X_C1* (user defined)

*X_C1 can not be selected as the y-axis variable

2

Enter minimum and maximum values, respectively, for: T(K)

903

1273

Enter minimum and maximum values, respectively, for: P(bar)

0.1

12000

For gridded minimization, grid resolution is determined by the number of levels (grid_levels) and the resolution at the lowest level in the X- and Y-directions (x_nodes and y_nodes) these parameters are currently set for the exploratory and autorefine cycles as follows:

stage	grid_levels	xnodes	ynodes	effective resolution
exploratory	1	40	40	40 x 40 nodes
auto-refine	4	60	60	473 x 473 nodes

To change these options edit or create the file perplex_option.dat

See: www.perplex.ethz.ch/perplex_options.html#grid_parameters

All thermodynamic components must be constrained, specify saturated components also (Y/N)?

n

Specify component amounts by mass (Y/N)?

n

The amounts you enter next need not be normalized; regardless of units, they define the molar amount of the system

Enter the molar amounts of the components:

Na2O MgO Al2O3 K2O CaO FeO H2O

for the bulk composition of interest:

1.94

12.74

30.66

9.83

0.97

23.74

22.39

Output a print file (Y/N)?

y

****warning ver056**** the EoS specified for H2O by the hybrid_EoS option will be overridden by the EoS specified in the problem definition file. To prevent this behavior set the GFSM option to True.

Exclude pure and/or endmember phases (Y/N)?

n

Include solution models (Y/N)?

Y

Enter the solution model file name [default = solution_model.dat]:

[enter]

...

Select models from the following list, enter 1 per line, press <enter> to finish

ternary-feldspar models: feldspar feldspar_B Pl(I1,HP) Fsp(C1)...

...

For details on these models see: www.perplex.ethz.ch/perplex_solution_model_glossary.html or read the commentary in the solution model file.

Bi(W)

Mica(W)

Gt(W)

St(W)

Crd(W)

Opx(W)

feldspar

melt(W)

Enter calculation title:

Ex12

(2) Doing the calculation (VERTEX)

Run VERTEX to make the calculation:

```
C:\PERPLEX\Perplex691>vertex
```

Perple_X version 6.9.1, source updated January 14, 2022.

Copyright (C) 1986-2022 James A D Connolly <www.perplex.ethz.ch/copyright.html>.

Enter the project name (the name assigned in BUILD) [default = my_project]:

ex12

...

(3) Plotting the calculated phase diagram (PSSECT)

Run PSSECT to plot the calculated pseudosection:

```
C:\PERPLEX\Perplex691>pssect
```

Perple_X version 6.9.1, source updated January 14, 2022.

Copyright (C) 1986-2022 James A D Connolly <www.perplex.ethz.ch/copyright.html>.

Enter the project name (the name assigned in BUILD) [default = my_project]:

ex12

Reading Perple_X options from: perplex_option.dat

Perple_X plot options are currently set as:

Keyword:	Value:	Permitted values [default]:
axis_label_scale	1.20	[1.2] (rel)
bounding_box :		
	0	[0] x-min (pts)
	0	[0] y-min (pts)
	800	[800] x-length (pts)
	800	[800] y-length (pts)
field_fill	T	[T] F
field_label	T	[T] F
numeric_field_label	F	[F] T, if T PSSECT writes list to *_assemblages.txt
replicate_label	0.250	0->1 [0.025]
field_label_scale	0.75	[0.72] (rel)
font	Helvetica	
grid	F	[F] T
half_ticks	T	[T] F
line_width	1.00	0-99 [1.] (pts)
picture_transformation :		
	0.180	[0.18] x-scale (rel)
	0.180	[0.18] y-scale (rel)

```

130. [0.18] x-translation (pts)
220. [0.18] y-translation (pts)
0.00 [0.0] rotation (deg)
plot_aspect_ratio 1.000 [1.0] x_axis_length/y_axis_length
splines          T      [T] F
tenth_ticks      F      [F] T
text_scale       1.000 [1.] (rel)
plot_extra_data

```

To change these options edit or create the plot option file

See: www.perplex.ethz.ch/perplex_plot_options.html

PostScript will be written to file: ex12.ps

Modify the default plot (y/n)?

n

There are 4 fields for: feldspar feldspar Bi(W) Mica(W) sill H2O

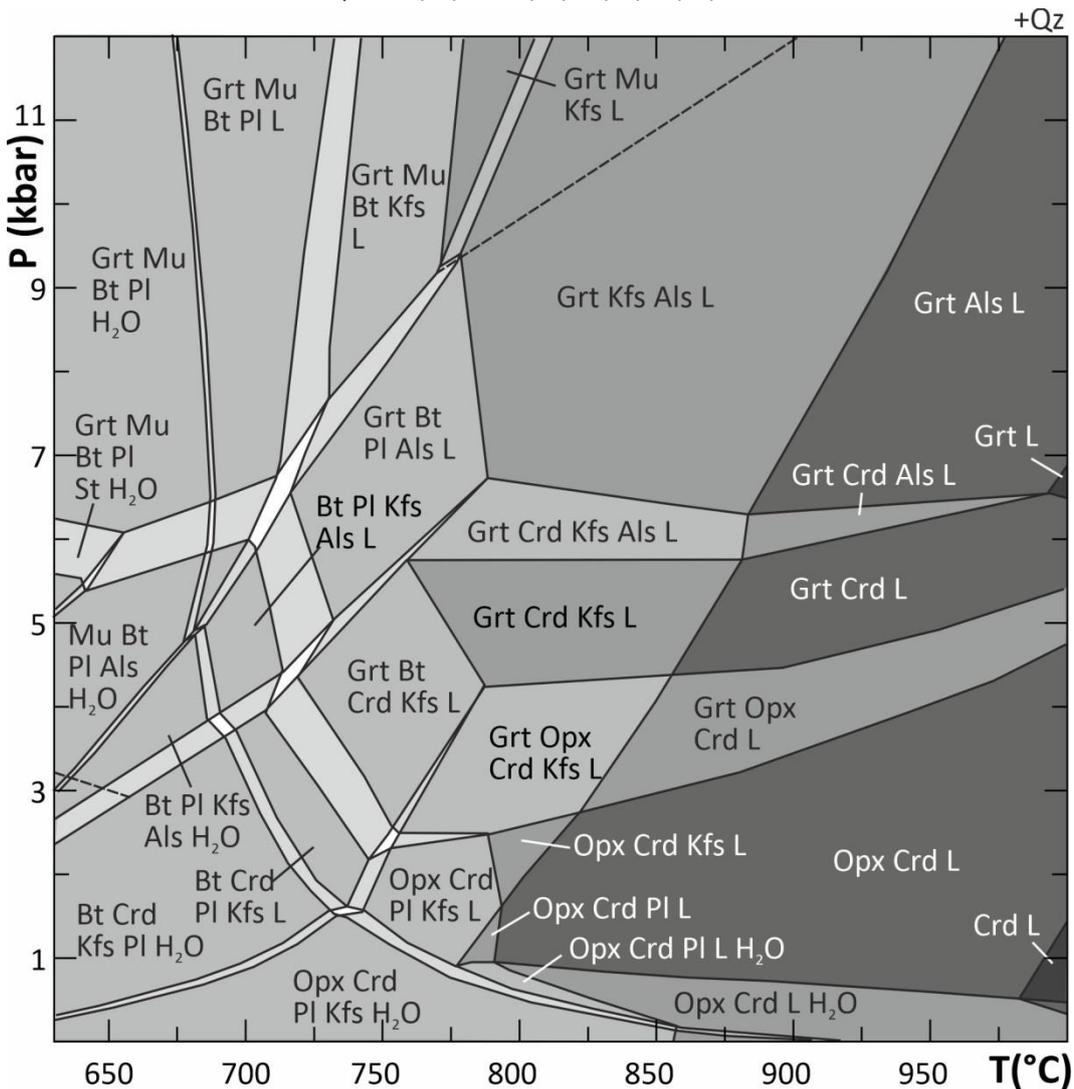
There are 8 fields for: Crd(W) Opx(W) feldspar feldspar Bi(W) H2O

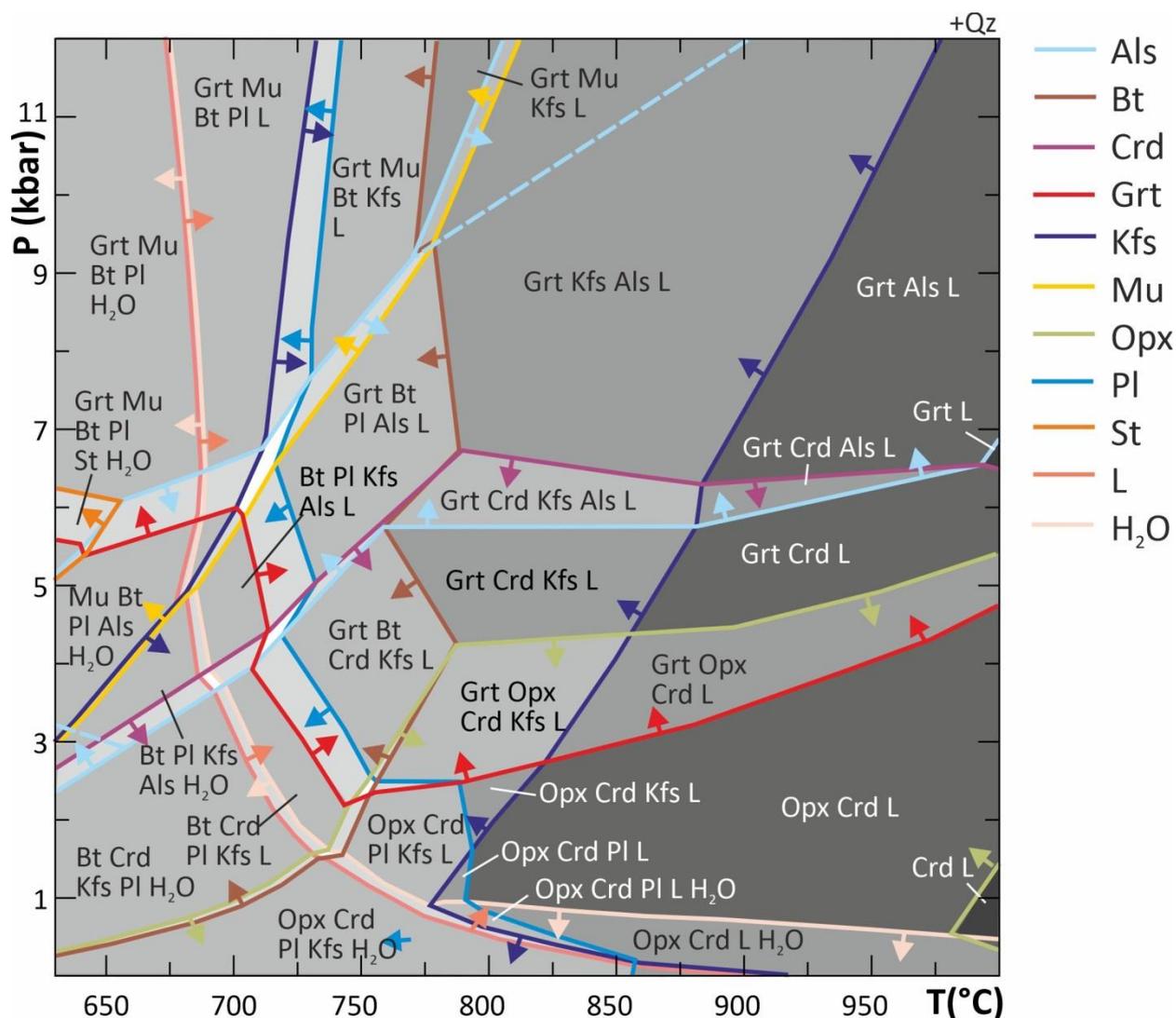
There are 13 fields for: melt(W) Opx(W) Crd(W) feldspar feldspar H2O

There are 2 fields for: melt(W) Opx(W) Crd(W) feldspar

There are 2 fields for: feldspar Bi(W) St(W) Mica(W) sill H2O

There are 2 fields for: feldspar Gt(W) Mica(W) St(W) Bi(W) sill H2O





(4) Calculating ISOMODES (WERAMI)

This section explains how to calculate the **variation in the modal amounts** of each phase (vol%) for the modelled pseudosection. There are also suggestions for calculating **isomodes for 2 immiscible phases (i.e. Pl and Kfs) of the same solution (i.e. feldspar) coexisting in one or more fields.**

Run WERAMI to calculate the ISOMODES of each phase.

```
C:\PERPLEX\Perplex691>werami
```

Perple_X version 6.9.1, source updated January 3, 2022.

Copyright (C) 1986-2022 James A D Connolly <www.perplex.ethz.ch/copyright.html>.

Enter the project name (the name assigned in BUILD) [default = my_project]:

```
ex12
```

Reading Perple_X options from: perplex_option.dat
Writing Perple_X option summary to: not requested

Perple_X computational option settings for WERAMI:

Keyword: Value: Permitted values [default]:

Input/Output options:

aqueous_output T [F] T
aqueous_species 20 [20] 0-150
aq_solvent_composition y [y] m: y => mol fraction, m => molality
aq_solute_composition m y [m]: y => mol fraction, m => molality
spreadsheet T [F] T
logarithmic_p F [F] T
bad_number NaN [NaN]
composition_constant F [F] T
composition_phase mol [mol] wt
composition_system wt [wt] mol
proportions vol [vol] wt mol
absolute F [F] T
cumulative F [F] T
fancy_cumulative_modes F [F] T
interpolation on [on] off
melt_is_fluid F [F] T
solution_names mod [model] abbreviation full
structural_formulae T [T] F
output_species T [T] F
output_species_props F [F] T
seismic_output som [some] none all
pause_on_error T [T] F
poisson_test F [F] T
interim_results aut [auto] off manual
sample_on_grid T [T] F
auto_exclude T [T] F

Information file output options:

option_list_files F [F] T; echo computational options

Thermodynamic options:

approx_alpha T [T] F
Anderson-Gruneisen F [F] T
hybrid_EoS_H2O 4 [4] 0-2, 4-7
hybrid_EoS_CO2 4 [4] 0-4, 7
hybrid_EoS_CH4 0 [0] 0-1, 7
fd_expansion_factor 2.0 [2] >0
finite_difference_p 0.1E+05 [1d4] >0; fraction = 0.1E-02 [1d-2]

Seismic wavespeed computational options:

seismic_data_file T [F] T
bounds VRH [VRH] HS
vrh/hs_weighting 0.5 [0.5] 0->1
explicit_bulk_modulus T [T] F
poisson_ratio on [on] all off; Poisson ratio = 0.35
seismic_output som [some] none all
poisson_test F [F] T

Tisza_test F [F] T

To change these options see: www.perplex.ethz.ch/perplex_options.html

warning ver056 the EoS specified for H2O by the hybrid_EoS option will be overridden by the EoS specified in the problem definition file. To prevent this behavior set the GFSM option to True.

Select operational mode:

- 1 - properties at specified conditions
- 2 - properties on a 2d grid
- 3 - properties along a 1d path
- 4 - as in 3, but input from file
- 0 - EXIT

2

Select a property:

- 1 - Specific Enthalpy (J/m³)
- 2 - Density (kg/m³)
- 3 - Specific heat capacity (J/K/m³)
- 4 - Expansivity (1/K, for volume)
- 5 - Compressibility (1/bar, for volume)
- 6 - Composition (Mol, Mass, or Wt%) of the system
- 7 - Mode (Vol, Mol, or Wt proportion) of a phase
- 8 - Composition (Mol, Mass, or Wt%) of a solution phase
- 9 - Grueneisen thermal ratio
- 10 - Adiabatic bulk modulus (bar)
- 11 - Adiabatic shear modulus (bar)
- 12 - Sound velocity (km/s)
- 13 - P-wave velocity (Vp, km/s)
- 14 - S-wave velocity (Vs, km/s)
- 15 - Vp/Vs
- 16 - Specific entropy (J/K/m³)
- 17 - Entropy (J/K/kg)
- 18 - Enthalpy (J/kg)
- 19 - Heat Capacity (J/K/kg)
- 20 - Specific mass of a phase (kg/m³-system)
- 21 - Poisson ratio
- 22 - Molar Volume (J/bar)
- 23 - Dependent potentials (J/mol, bar, K)
- 24 - Assemblage Index
- 25 - Modes of all phases
- 26 - Sound velocity T derivative (km/s/K)
- 27 - P-wave velocity T derivative (km/s/K)
- 28 - S-wave velocity T derivative (km/s/K)
- 29 - Adiabatic bulk modulus T derivative (bar/K)
- 30 - Shear modulus T derivative (bar/K)
- 31 - Sound velocity P derivative (km/s/bar)
- 32 - P-wave velocity P derivative (km/s/bar)
- 33 - S-wave velocity P derivative (km/s/bar)
- 34 - Adiabatic bulk modulus P derivative (unitless)
- 35 - Shear modulus P derivative (unitless)

- 36 - All phase &/or system properties
- 37 - Absolute amount (Vol, Mol, or Wt) of a phase
- 38 - Multiple property output
- 39 - Heat capacity ratio (Cp/Cv)
- 40 - Lagged or back-calculated aqueous solute chemistry

7

Enter solution or compound (left justified):

melt(W)

Include fluid in computation of aggregate (or modal) properties (y/n)?

n

Fractions are Wt, Vol, or Mol depending on the perplex_option.dat proportions keyword.

Select an additional property or enter 0 to finish:

7

Enter solution or compound (left justified):

Mica(W)

Include fluid in computation of aggregate (or modal) properties (y/n)?

n

Fractions are Wt, Vol, or Mol depending on the perplex_option.dat proportions keyword.

Select an additional property or enter 0 to finish:

7

Enter solution or compound (left justified):

Bi(W)

Include fluid in computation of aggregate (or modal) properties (y/n)?

n

Fractions are Wt, Vol, or Mol depending on the perplex_option.dat proportions keyword.

Select an additional property or enter 0 to finish:

7

Enter solution or compound (left justified):

feldspar

Include fluid in computation of aggregate (or modal) properties (y/n)?

n

Fractions are Wt, Vol, or Mol depending on the perplex_option.dat proportions keyword.

Select an additional property or enter 0 to finish:

7

Enter solution or compound (left justified):

Gt(W)

Include fluid in computation of aggregate (or modal) properties (y/n)?

n

Fractions are Wt, Vol, or Mol depending on the perplex_option.dat proportions keyword.

Select an additional property or enter 0 to finish:

7

Enter solution or compound (left justified):

Crd(W)

Include fluid in computation of aggregate (or modal) properties (y/n)?

n

Fractions are Wt, Vol, or Mol depending on the perplex_option.dat proportions keyword.

Select an additional property or enter 0 to finish:

7

Enter solution or compound (left justified):

Opx(W)

Include fluid in computation of aggregate (or modal) properties (y/n)?

n

Fractions are Wt, Vol, or Mol depending on the perplex_option.dat proportions keyword.

Select an additional property or enter 0 to finish:

7

Enter solution or compound (left justified):

ky

Include fluid in computation of aggregate (or modal) properties (y/n)?

n

Fractions are Wt, Vol, or Mol depending on the perplex_option.dat proportions keyword.

Select an additional property or enter 0 to finish:

7

Enter solution or compound (left justified):

sill

Include fluid in computation of aggregate (or modal) properties (y/n)?

n

Fractions are Wt, Vol, or Mol depending on the perplex_option.dat proportions keyword.

Select an additional property or enter 0 to finish:

7

Enter solution or compound (left justified):

and

Include fluid in computation of aggregate (or modal) properties (y/n)?

n

Fractions are Wt, Vol, or Mol depending on the perplex_option.dat proportions keyword.

Select an additional property or enter 0 to finish:

0

Change default variable range (y/n)?

n

Select the grid resolution (to use an arbitrary grid set sample_on_grid to F):

1 - 60 x 60 nodes

2 - 119 x 119 nodes

3 - 237 x 237 nodes

4 - 473 x 473 nodes [default]

4

...
...

2 immiscible phases of feldspar coexist with the following molar compositions:

H2O	MgO	Al2O3	K2O	CaO	FeO	Na2O	SiO2
0.000	0.000	0.789	0.009	0.577	0.000	0.202	2.423
0.000	0.000	0.505	0.422	0.010	0.000	0.073	2.990

Identify the phase of interest by:

- 1 - the maximum value of a composition [default].
- 2 - the minimum value of a composition.
- 3 - the range of one or more compositions.
- 4 - a combination of the above.
- 5 - average the compositions of immiscible phases.

Kfs and Pl have been modelled using the same solid solution model ("feldspar"); therefore, in the modelled pseudosection, you have fields in which two feldspars coexist. For those fields where there are two stable feldspars, you should specify what do you want to calculate (i.e. isomodes for Kfs or for Pl?).

You should choose one of the above criteria: for example, if you want to calculate the isomodes for plagioclase, you can specify that the phase of interest should be identified based on the maximum anorthite content (and, conversely, if you want to calculate the isomodes for K-feldspar, it should be identified based on the maximum sanidine content, or the minimum anorthite content).

1

The following prompts define the composition C[1] to be used to identify the phase of interest.

NOTE: discriminatory criteria are only applied when immiscible phases coexist. If only one phase of a solution is stable, then data for this phase is output regardless of whether the phase meets the criteria specified here.

Read carefully this note.

Define the composition in terms of the species/endmembers of feldspar (y/n)?

Answer no to define a composition in terms of the systems components. Units (mass or molar) are controlled by the composition keyword in perplex_option.dat.

y

Compositions are defined as a ratio of the form:

$$\text{Sum } \{w(i)*n(i), i = 1, c1\} / \text{Sum } \{w(i)*y(i), i = c2, c3\}$$

y(j) = mole fraction of species j

w(j) = weighting factor of species j (usually 1)

How many components in the numerator of the composition (<13)?

1

Enter species indices and weighting factors for the numerator:

- 1 - abh
- 2 - an
- 3 - san

2
1

How many species in the denominator of the composition (<12)?
Enter zero to use the numerator as a composition.

0

The compositional variable is: 1.0 an
Change it (y/n)?

n

Remember that you are calculating the isomodes of plagioclase in those fields where two feldspar coexist. In the fields where you have only one feldspar, the calculated isomodes refer to either Pl or Kfs, depending on which one is stable.

In order to calculate the isomodes of K-feldspar in the fields where two feldspar coexists, you should run again WERAMI, asking for Kfs isomodes.

****warning ver637**** Immiscibility occurs in one or more phases. Interpolation will be turned off at all affected nodes. override this feature at the risk of computing inconsistent properties by setting the option `warning_ver637` to F and restarting WERAMI.

Data ranges excluding values equal to `bad_number` (NaN) specified in `perplex_option.dat`:

	melt(W),vo%	Mica(W),vo%	Bi(W),vo%	feldspar,vo%	Gt(W),vo%	Crd(W),vo%	Opx(W),vo%	ky,vo%
min	0.156117E-001	0.933335E-003	0.220004E-003	0.176996E-003	0.163138E-003	0.202035E-003	0.177261E-003	0.113827E-001
max	86.7425	55.0618	56.1606	50.0475	29.3697	39.7275	13.1724	5.06174
	16.5593							16.2232

Output has been written to the 2d tab format file: `ex12_1.tab`

2d tab format files can be processed with:

- PSTABLE - a Perple_X plotting program
- PERPLE_X_PLOT - a MATLAB plotting script
- PYWERAMI - github.com/ondrolexa/pywerami
- spread-sheet programs, e.g., EXCEL

for details on tab format refer to:

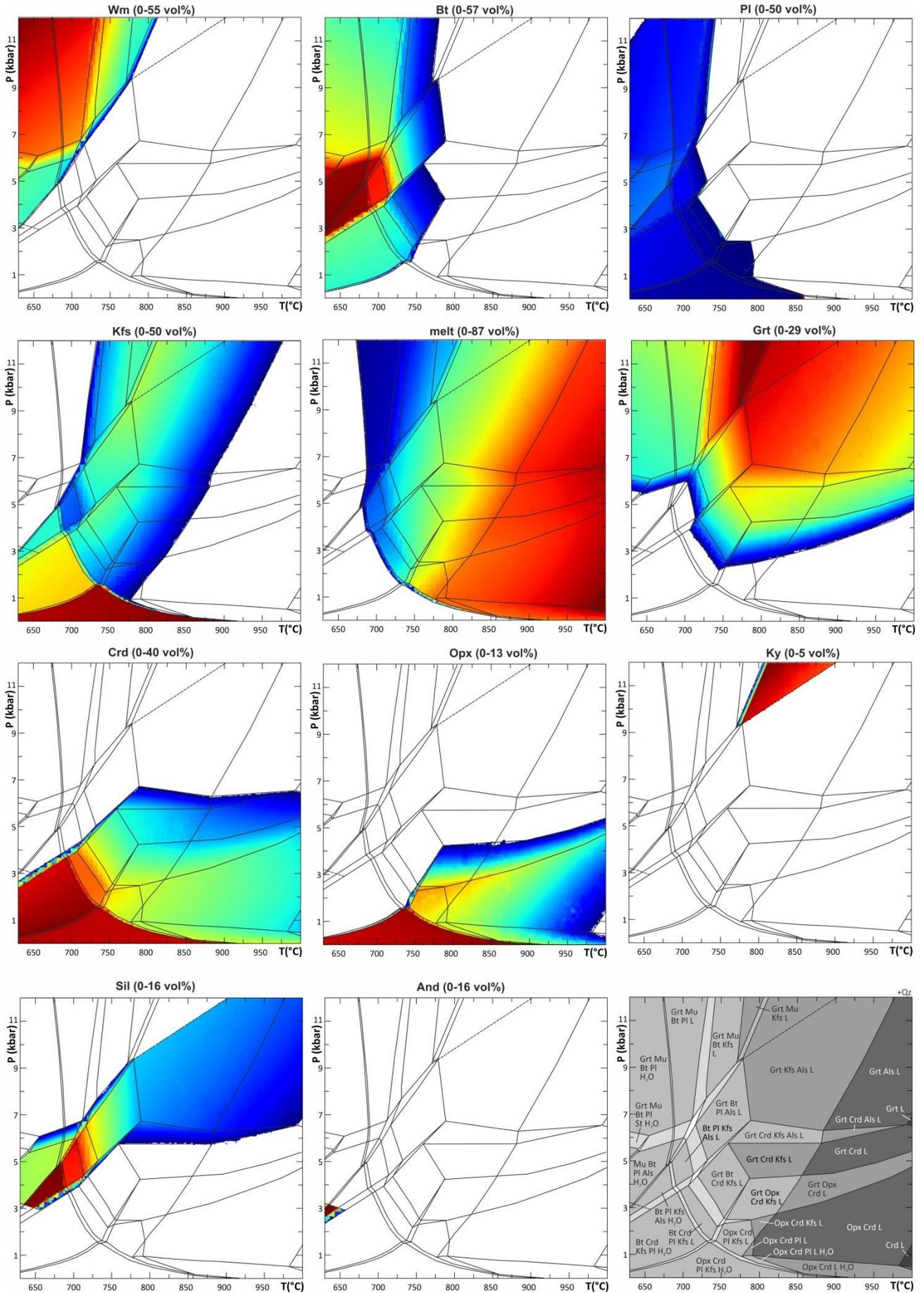
perplex.ethz.ch/perplex/faq/Perple_X_tab_file_format.txt

Select operational mode:

- 1 - properties at specified conditions
- 2 - properties on a 2d grid
- 3 - properties along a 1d path
- 4 - as in 3, but input from file
- 0 - EXIT

0

At the end, you have a new file (`ex12_1.tab`) in the `Perple_X` folder.
Run again WERAMI to calculate isomodes for K-feldspar (`ex12_2.tab`).



NB: If you have doubts on which feldspar is stable in each field assemblage, you can run WERAMI, option 1. This option allows to calculate all the properties of the system (including phase compositions) at specified P-T conditions.

For example at **973 K (700°C), 8 kbar:**

Stable phases at:

T(K) = 973.000
P(bar) = 8000.00

Phase Compositions (molar proportions):

	wt %	vol %	mol %	mol	H2O	MgO	Al2O3	K2O	CaO	FeO	Na2O	SiO2
Bi(W)	30.27	30.16	25.03	7.84	1.00000	1.20981	0.79551	0.50000	0.00000	1.49469	0.00000	2.70449
feldspar	6.61	7.64	9.56	2.99	0.00000	0.00000	0.58328	0.02486	0.16657	0.00000	0.39186	2.83343
Gt(W)	19.14	14.05	15.34	4.81	0.00000	0.54150	1.00000	0.00000	0.08679	2.37171	0.00000	3.00000
melt(W)	2.76	3.92	10.30	3.23	0.65030	0.00118	0.13549	0.04215	0.00403	0.00378	0.08085	1.12957
Mica(W)	41.22	44.23	39.77	12.5	1.00000	0.05226	1.40002	0.45771	0.00331	0.04937	0.04063	3.09832

Phase speciation (molar proportions):

Bi(W) east: 0.29551, ann: 0.51681, phl: 0.24344, obi: -0.05576

feldspar abh: 0.78371, an: 0.16657, san: 0.04972

Gt(W) alm: 0.79057, py: 0.18050, gr: 0.02893

melt(W) fo8L: 0.00030, fa8L: 0.00094, abL: 0.16171, sil8L: 0.00528, anL: 0.00403, kspL: 0.08430, q8L: 0.09314
h2oL: 0.65030

Mica(W) mu: 0.81379, pa: 0.08126, ma1_dqf: 0.00331, cel: 0.05226, fcel: 0.04937

Ex 13

Ex. 13 – INDIRECT modelling of an anatectic METAPELITE

In Ex. 12 we have considered a model metapelite, and we have supposed to know the protolith bulk composition (including its initial H₂O amount). However, **in most cases, we have to deal with natural samples, of which we do not know the whole history.** Furthermore, **a number of evidence are consistent with most migmatites and granulites having lost some to virtually all of their melt during metamorphism.**

This exercise aims at modelling a REAL SAMPLE OF ANATECTIC METAPELITE.

What do we know?

- The observed mineral assemblage
- The measured mineral compositions
- The measured bulk composition (which often does not coincide with the composition of the protolith!)

What we do not know?

- The bulk composition of the protolith (if a certain amount of melt was lost during the prograde evolution)
- The amount of melt that was lost
- The number of melt loss events
- The P-T conditions at which melt was lost

STRATEGY

The problem can be divided in two parts:

- (A)** If a certain amount of melt was lost during the prograde evolution, the measured bulk composition of the sample represents the **FINAL** rock composition, after the loss of that melt. Therefore, the pseudosection calculated using the **MEASURED bulk composition** allows to constrain the **P-T evolution from peak conditions to final melt crystallization (i.e. retrograde evolution)**, but may not be valid for the prograde evolution of the rock.
- (B)** An **APPROXIMATE PROTOLITH COMPOSITION** can be calculated by **REINTEGRATING** melt into the measured rock composition. The pseudosection calculated using the **MELT-REINTEGRATED bulk composition** allows the exploration of the extended supra-*solidus* domain and the assessment of an **APPROXIMATE prograde evolution.**

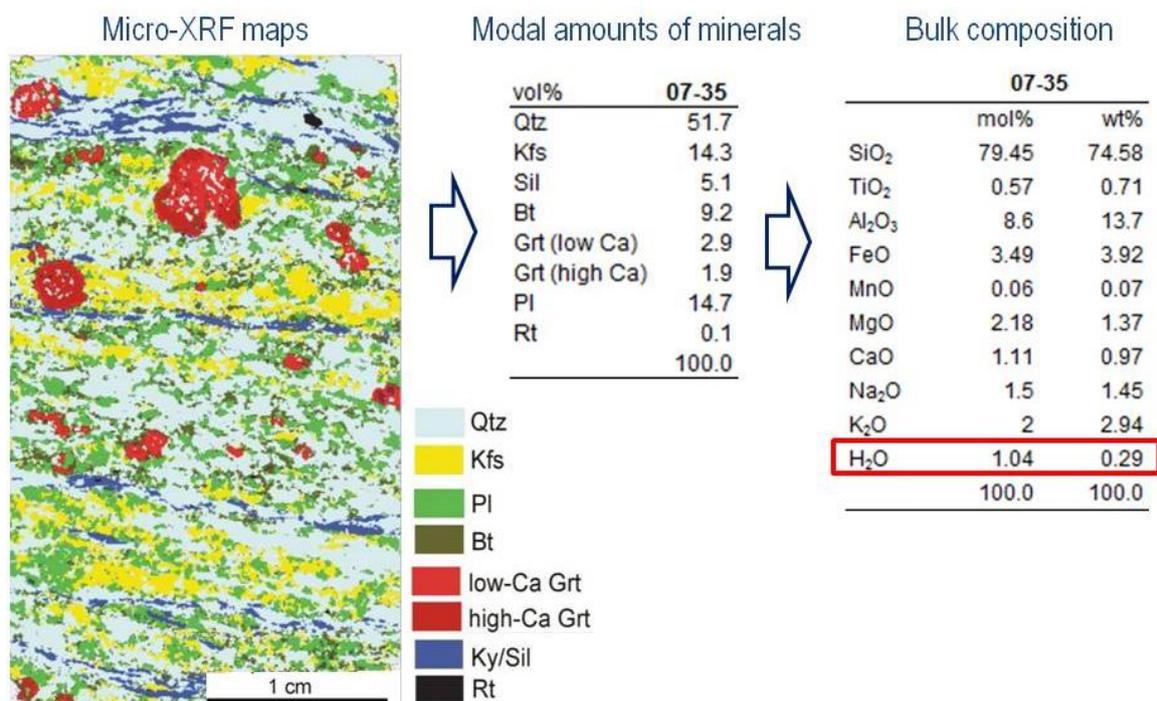
Ex. 13.1 – P-T EVOLUTION from PEAK conditions to FINAL MELT CRYSTALLIZATION

This exercise is based on the paper by Groppo et al. (2012) [J. Petrol., 53, 1057-1088]. The P-T pseudosection is reported in their Fig. 10a.

MEASURED BULK COMPOSITION

Bulk composition may be obtained using conventional methods (e.g. XRF, ICP-MS), **BUT** we need a precise estimate of the H₂O amount in the bulk. A **PRECISE ESTIMATE OF THE H₂O CONTENT IN THE BULK** is, in fact, crucial because it controls the position of the *solidus* and the amount of melt that can be produced from the source rock as a function of P-T. **Conventional methods do not provide such an accurate estimate of H₂O content (do not thrust the LOI value!).**

My suggested method is to combine the mineral proportions obtained from the modal estimate of an X-ray compositional map of the whole thin section with the mineral chemistry acquired at the microprobe. This method allows a precise estimate of the modal percentage of hydrous minerals (e.g. biotite, cordierite) in the rock, which is required to derive the H₂O content in the bulk.



(1) Definition of the problem (BUILD)

Bulk composition (mol%):

SiO₂=79.45; TiO₂: 0.57; Al₂O₃=8.6, FeO=3.49, MgO=2.18, CaO=1.11, Na₂O=1.5, K₂O=2.00, H₂O=1.04

T=700-900°C

P=3-15 kbar

Because the problem is similar to that of Ex. 12, we can try to skip the BUILD session and to directly edit the input file, starting from that of Ex. 12 (Use the perplex option `ex12.dat` file created for Ex12).

NB: SiO₂ is not considered in excess; add TiO₂ in the list of thermodynamic components; change the P-T range of interest.

(2) Doing the calculation (VERTEX)

Run vertex to make the calculation:

```
C:\PERPLEX\Perplex691>vertex
```

```
Perple_X version 6.9.1, source updated January 14, 2022.
```

```
Copyright (C) 1986-2022 James A D Connolly <www.perplex.ethz.ch/copyright.html>.
```

```
Enter the project name (the name assigned in BUILD) [default = my_project]:
```

```
ex13
```

```
...
```

(3) Plotting the calculated phase diagram (PSSECT)

Run PSSECT to plot the calculated pseudosection:

```
C:\PERPLEX\Perplex691>pssect
```

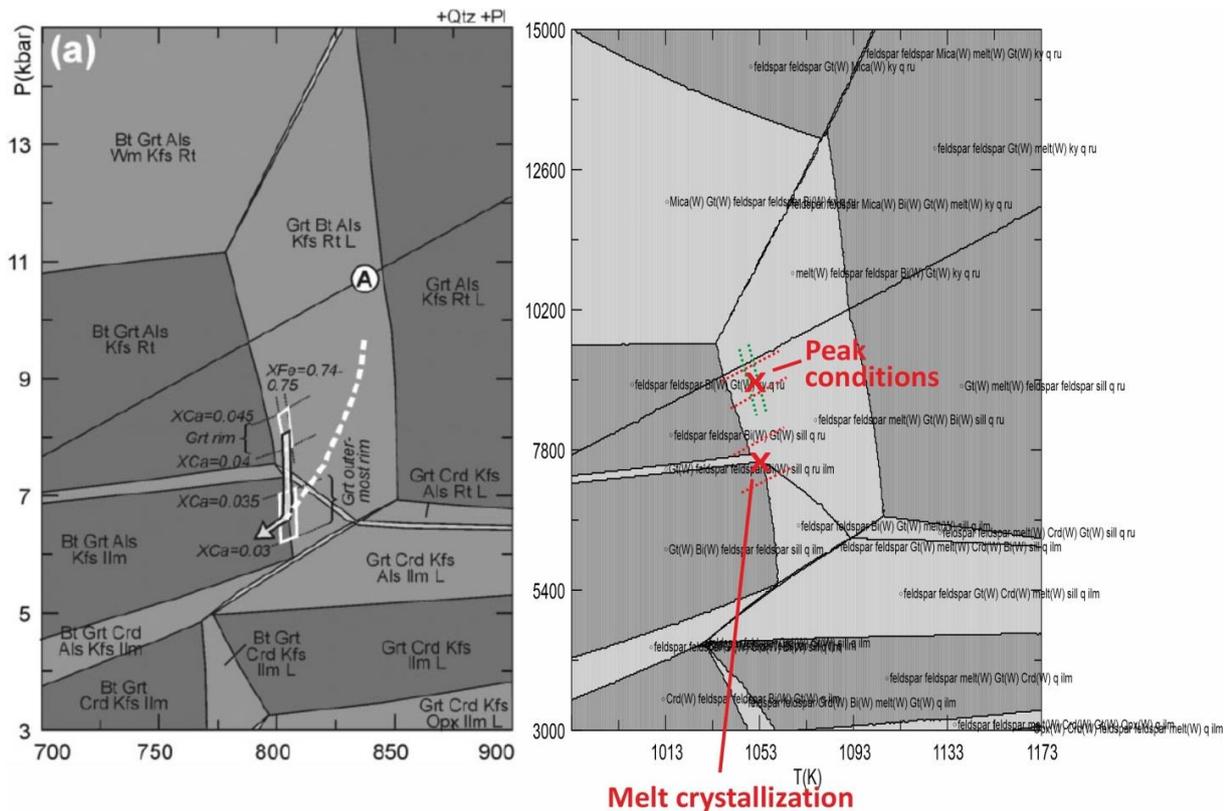
```
Perple_X version 6.9.1, source updated January 14, 2022.
```

```
Copyright (C) 1986-2022 James A D Connolly <www.perplex.ethz.ch/copyright.html>.
```

```
Enter the project name (the name assigned in BUILD) [default = my_project]:
```

```
ex13
```

```
...
```

Comparison with Fig. 10a in Groppo et al. (2012). Note that, although minor changes occur in the topology of the pseudosection due to the different thermodynamic databases and solid solution models used, the final results are very similar.

Option 1 of WERAMI allows to quickly check if the modelled mineral modes at the *solidus* (i.e. at P-T conditions estimated for the final melt crystallization: 780°C, 7 kbar) are comparable (within the error) with the observed mineral modes.

Werami, option 1

Stable phases at:

T(K) = 1053.00
P(bar) = 7500.00

Phase Compositions (molar proportions):

	wt %	vol %	mol %	mol	H2O	TiO2	Na2O	MgO	Al2O3	K2O	CaO	FeO	SiO2
Gt(W)	5.31	3.56	1.13	0.717	0.00000	0.00000	0.00000	0.71637	1.00000	0.00000	0.09340	2.19024	3.00000
Bi(W)	9.40	8.44	2.05	1.30	0.79760	0.20240	0.00000	1.27785	0.78270	0.50000	0.00000	1.23705	2.71730
feldspar	14.02	14.94	5.13	3.27	0.00000	0.00000	0.11742	0.00000	0.51228	0.37030	0.02456	0.00000	2.97544
feldspar	14.55	15.06	5.46	3.47	0.00000	0.00000	0.32147	0.00000	0.63861	0.03992	0.27722	0.00000	2.72278
sill	7.53	6.32	4.67	2.97	0.00000	0.00000	0.00000	0.00000	1.00000	0.00000	0.00000	0.00000	1.00000
q	48.47	51.26	81.09	51.6	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	1.00000
ilm	0.73	0.42	0.48	0.306	0.00000	1.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	1.00000

Mineral modes

780°C, 7.5 kbar

	observed	modelled
Qtz	51.7	51.3
Kfs	14.3	15.0
Sil	5.1	6.3
Bt	9.2	8.4
Grt	4.8	3.6
Pl	14.7	14.9

Ex. 13.2 – PROGRADE P-T EVOLUTION and MELT RE-INTEGRATION

This exercise is based on the paper by Groppo et al. (2012) [J. Petrol., 53, 1057-1088]. The P-T pseudosection is reported in their Fig. 10b.

In natural systems, it is not possible to know exactly the total amount and composition of missing melt and the number of episodes of melt loss, therefore the EXACT missing melt cannot be added back to reconstruct the real sub-*solidus* protolith composition. As a consequence, **the prograde portion of the P-T evolution of anatectic rocks is generally less well constrained than the retrograde one.**

An APPROXIMATE protolith composition can be calculated by reintegrating melt into the measured bulk rock composition. It has been demonstrated that the simple case of a **single event of melt loss (occurred at peak T conditions)** is a defensible end-member case.

(i) How much melt should be re-integrated?

An amount of melt sufficient to model a H₂O-saturated *solidus* in the pressure range of interest.

This melt-reintegrated composition likely approximates that of a protolith containing the maximum possible amount of mica before melting.

How to calculate the amount of melt to be reintegrated?

Use a **trial and error method.**

- start from the measured bulk composition and add a small amount of melt (e.g. 5% of melt); calculate a new pseudosection with the reintegrated bulk composition (better if you extend the T range down to 650°C); check if the modelled *solidus* is still dry or wet.
- repeat this process until a H₂O-saturated (wet) *solidus* is modelled in the P-range of interest.

(ii) Of which composition?

The composition of reintegrated melt can be calculated at peak-T conditions.

How to estimate the melt composition to be reintegrated?

Run WERAMI, option 1, at peak P-T conditions. The melt composition is expressed in molar proportions of oxides (see below).

Run Werami, option 1 **to estimate the melt composition at peak T conditions** (780°C, 9.0 kbar)

Stable phases at:

T(K) = 1053.00

P(bar) = 9000.00

Phase Compositions (molar proportions):

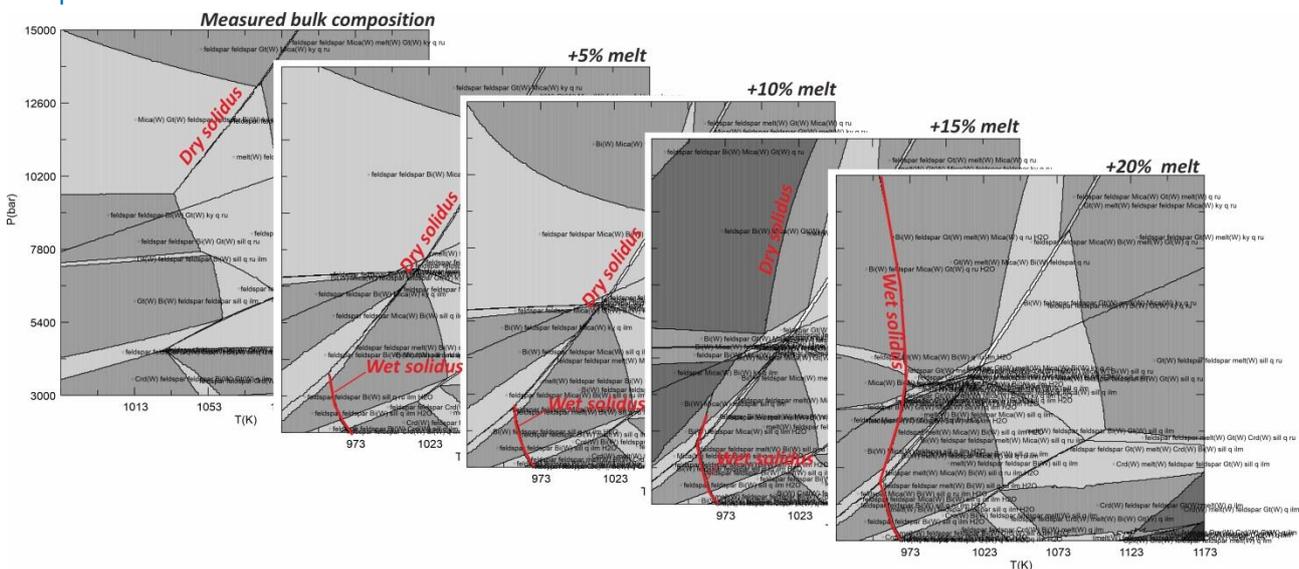
	wt %	vol %	mol %	mol	H2O	TiO2	Na2O	MgO	Al2O3	K2O	CaO	FeO	SiO2
feldspar	15.60	16.70	5.77	3.63	0.00000	0.00000	0.11353	0.00000	0.51211	0.37436	0.02423	0.00000	2.97577
feldspar	13.60	14.15	5.16	3.25	0.00000	0.00000	0.32370	0.00000	0.63549	0.04081	0.27099	0.00000	2.72901
melt(W)	0.96	1.20	0.79	0.500	0.56926	0.00000	0.07162	0.00202	0.17425	0.07194	0.01173	0.00563	1.38010
Gt(W)	8.43	5.70	1.82	1.14	0.00000	0.00000	0.00000	0.77017	1.00000	0.00000	0.11873	2.11110	3.00000
Bi(W)	6.74	6.12	1.50	0.942	0.80152	0.19848	0.00000	1.37838	0.78303	0.50000	0.00000	1.14011	2.71697
sill	6.86	5.79	4.30	2.71	0.00000	0.00000	0.00000	0.00000	1.00000	0.00000	0.00000	0.00000	1.00000
q	47.32	50.01	80.05	50.4	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	1.00000
ru	0.48	0.31	0.61	0.383	0.00000	1.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000

Calculate the re-integrated bulk compositions adding small amounts of melt to the measured bulk composition.

	melt composition (790°C, 9.0 kbar)		BC**	Melt reintegrated bulk compositions							
	mol*	mol%		mol%	+5% melt		+10% melt		+15% melt		+20% melt
SiO2	1.3801	60.36	79.45	82.5	78.54	85.5	77.71	88.5	76.96	91.5	76.27
TiO2	0.0000	0.00	0.57	0.6	0.54	0.6	0.52	0.6	0.50	0.6	0.48
Al2O3	0.1743	7.62	8.60	9.0	8.55	9.4	8.51	9.7	8.47	10.1	8.44
FeO	0.0056	0.25	3.49	3.5	3.34	3.5	3.20	3.5	3.07	3.5	2.95
MnO	0.0000	0.00	0.06	0.1	0.06	0.1	0.05	0.1	0.05	0.1	0.05
MgO	0.0020	0.09	2.18	2.2	2.08	2.2	1.99	2.2	1.91	2.2	1.83
CaO	0.0117	0.51	1.11	1.1	1.08	1.2	1.06	1.2	1.03	1.2	1.01
Na2O	0.0716	3.13	1.50	1.7	1.58	1.8	1.65	2.0	1.71	2.1	1.77
K2O	0.0719	3.15	2.00	2.2	2.05	2.3	2.10	2.5	2.15	2.6	2.19
H2O	0.5693	24.90	1.04	2.3	2.18	3.5	3.21	4.8	4.15	6.0	5.02
Total	2.2866	100.00	100	105.0	100.00	110.0	100.00	115.0	100.00	120.0	100.00

* this composition has been obtained using WERAMI 1 for the pseudosection calculated using the actually measured bulk composition

Start adding a small amount of melt (+5% melt); use the new “melt-reintegrated” bulk composition to calculate a new pseudosection and check if the *solidus* is dry or wet. Repeat this process for progressively increasing amounts of melt reintegrated to the measured bulk composition and check the nature of the *solidus* each time.



The pseudosection calculated using the bulk composition obtained by re-integration of 20% of melt predicts a wet *solidus* over the entire pressure range of interest. This “melt-reintegrated” bulk composition should be therefore considered as the APPROXIMATE protolith composition.

You can use this “melt-reintegrated” pseudosection:

- (a) to constrain the APPROXIMATE prograde evolution of your sample and,
- (b) to estimate the MAXIMUM amount of melt that would have been produced if no melt loss occurred during the prograde evolution (i.e. if melt loss occurred in a single event, at peak P-T conditions).