ÚLOHA 2: vynesení izoplet módů fází a jejich složení do P-T diagramu

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Microsoft Windows XP [Verze 6.0.6002]
(C) Copyright 1985-2001 Microsoft Corp.

C:\Users\Terezka\Documents\Perple_X clear>werami

Perple_X version 6.7.0, source updated July 2, 2014.

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

Reading computational options from: perplex_option.dat
Writing computational option summary to file: not requested

Perple_X computational option settings for WERAMI:

   Keyword:              Value:     Permitted values [default]:

  Input/Output options:

   spreadsheet           T          [F] T
   logarithmic_p         F          [F] T
   bad_number            NaN        [0.0]
   composition           mol        wt  [mol]
   proportions           mol        wt  [vol] mol
   interpolation         on         off [on ]
   melt_is_fluid         F          [F] T
   seismic_output        som        none [some] all

  Information file output options:

   option_list_files     F          [F] T; echo computational options

  Thermodynamic options:

   approx_alpha          T          [T] F
   Anderson-Gruneisen    F          [T] F

  Seismic velocity options:

   bounds                VRH        HS  [VRH]
   vrh/hs_weighting      0.5        0->1 [0.5]
   explicit_bulk_modulus T          [F] T
   poisson_ratio         on         off [on ] all; Poisson ratio = 0.35

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 [enter 0 to finish]:
  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 or Wt%) of the system
  7 - Mode (Vol, Mol, or Wt proportion) of a phase
  8 - Composition (Mol 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)
25

Output cumulative modes (y/n)?
(see www.perplex.ethz.ch/perplex_options.html#cumulative_modes)
n

Change default variable range (y/n)?
n

Enter number of nodes in the X(C1) and T(K) directions:
200 200

warning ver178 at T(K)= 1373. P(bar)= 2000. the shear modulus of: abh
is missing or invalid and has been estimated from the default poisson ratio

warning ver178 at T(K)= 1373. P(bar)= 2000. the shear modulus of: Fsp(C1)
is missing or invalid and has been estimated from the default poisson ratio

warning ver637 Immiscibility occurs in one or more phases
interpolation will be turned off at all affected nodes.
To overide this feature at the risk of computing inconsistent properties
set solvus_tolerance = 1 and rerun VERTEX

warning ver178 at T(K)= 1376. P(bar)= 2000. the shear modulus of: abh
is missing or invalid and has been estimated from the default poisson ratio

warning ver178 at T(K)= 1376. P(bar)= 2000. the shear modulus of: Fsp(C1)
is missing or invalid and has been estimated from the default poisson ratio

warning ver178 at T(K)= 1379. P(bar)= 2000. the shear modulus of: abh
is missing or invalid and has been estimated from the default poisson ratio

warning ver178 at T(K)= 1379. P(bar)= 2000. the shear modulus of: Fsp(C1)
is missing or invalid and has been estimated from the default poisson ratio

warning ver178 at T(K)= 1382. P(bar)= 2000. the shear modulus of: abh
is missing or invalid and has been estimated from the default poisson ratio

warning ver178 at T(K)= 1382. P(bar)= 2000. the shear modulus of: Fsp(C1)
is missing or invalid and has been estimated from the default poisson ratio

warning ver178 at T(K)= 1385. P(bar)= 2000. the shear modulus of: abh
is missing or invalid and has been estimated from the default poisson ratio

warning ver178 at T(K)= 1385. P(bar)= 2000. the shear modulus of: Fsp(C1)
is missing or invalid and has been estimated from the default poisson ratio

warning ver178 at T(K)= 1388. P(bar)= 2000. the shear modulus of: abh
is missing or invalid and has been estimated from the default poisson ratio

warning ver049 warning 178 will not be repeated for future instances of this problem.
currently in routine: GETPHP

Data ranges excluding values equal to bad_number (NaN) specified in
perplex_option.dat:

	abh	melt(HP)	Fsp(C1)	Fsp(C1)
min	0.000000	0.000000	0.000000	0.000000
max	100.0000	100.0000	100.0000	93.73439

Output has been written to the 2d tab format file: ab_an_melt_7.tab

2d tab format files can be processed with:

PSTABLE - a Perple_X plotting program
PERPLE_X_PLOT - a MATLAB plotting script
PYWERAMI - petrol.natur.cuni.cz/~ondro/pywerami:home
spread-sheet programs, e.g., EXCEL

for details on tab format refer to:
perplex.ethz.ch/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
2

Select a property [enter 0 to finish]:
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 or Wt%) of the system
7 - Mode (Vol, Mol, or Wt proportion) of a phase

```
 8 - Composition (Mol 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)
8

Enter solution or compound name (left justified):
Fsp(C1)

Compositions are defined as a ratio of the form:
    Sum {w(i)*n(i), i = 1, c1} / Sum {w(i)*n(i), i = c2, c3}
            n(j) = mole proportion of component j
            w(j) = weighting factor of component j (usually 1)

How many components in the numerator of the composition (<13)?
1

Enter component indices and weighting factors for the numerator:
  1 - ab
  2 - an
1 1
```

How many components in the denominator of the composition (<12)?
Enter zero to use the numerator as a composition.
2

Enter component indices and weighting factors for the denominator:
  1 - ab
  2 - an
1 1
2 1

The compositional variable is:

1.0 ab

  divided by

1.0 ab + 1.0 an

Change it (y/n)?
n

This composition will be designated: C1Fsp(C1)

Select a property [enter 0 to finish]:
8

Enter solution or compound name (left justified):
melt(HP)

Compositions are defined as a ratio of the form:
  Sum {w(i)*n(i), i = 1, c1} / Sum {w(i)*n(i), i = c2, c3}
    n(j) = mole proportion of component j
    w(j) = weighting factor of component j (usually 1)

How many components in the numerator of the composition (<13)?
1

Enter component indices and weighting factors for the numerator:
  1 - ab
  2 - an
2 1

How many components in the denominator of the composition (<12)?
Enter zero to use the numerator as a composition.
2

Enter component indices and weighting factors for the denominator:
  1 - ab
  2 - an

1 1
2 1

The compositional variable is:

1.0 an

divided by

1.0 ab + 1.0 an

Change it (y/n)?
n

This composition will be designated: C2melt(HP)

Select a property [enter 0 to finish]:
0

Change default variable range (y/n)?
n

Enter number of nodes in the X(C1) and T(K) directions:
200 200

2 immiscible phases of Fsp(C1)
coexist with the following molar compositions:

ab	an
0.000	1.000
0.054	0.946

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.
5

Data ranges excluding values equal to bad_number (NaN) specified in perplex_option.dat:

	C1Fsp(C1)	C2melt(HP)
min	0.000000	0.000000
max	1.000000	1.000000

Output has been written to the 2d tab format file: ab_an_melt_8.tab

2d tab format files can be processed with:

PSTABLE - a Perple_X plotting program
PERPLE_X_PLOT - a MATLAB plotting script
PYWERAMI - petrol.natur.cuni.cz/~ondro/pywerami:home
spread-sheet programs, e.g., EXCEL

for details on tab format refer to:
perplex.ethz.ch/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

C:\Users\Terezka\Documents\Perple_X clear>

ÚLOHA 3: módy a složení fází podél linie

Microsoft Windows XP [Verze 6.0.6002]
(C) Copyright 1985-2001 Microsoft Corp.

C:\Users\Terezka\Documents\Perple_X clear>werami

Perple_X version 6.7.0, source updated July 2, 2014.

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

Reading computational options from: perplex_option.dat
Writing computational option summary to file: not requested

Perple_X computational option settings for WERAMI:

Keyword:	Value:	Permitted values [default]:
Input/Output options:		
spreadsheet	T	[F] T
logarithmic_p	F	[F] T
bad_number	NaN	[0.0]
composition	mol	wt [mol]
proportions	mol	wt [vol] mol

```
   interpolation          on        off [on ]
   melt_is_fluid          F         [F] T
   seismic_output         som       none [some] all

  Information file output options:

   option_list_files      F         [F] T; echo computational options

  Thermodynamic options:

   approx_alpha           T         [T] F
   Anderson-Gruneisen     F         [T] F

  Seismic velocity options:

   bounds                 VRH       HS  [VRH]
   vrh/hs_weighting       0.5       0->1 [0.5]
   explicit_bulk_modulus  T         [F] T
   poisson_ratio          on        off [on ] all; Poisson ratio = 0.35

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
3

Construct a non-linear profile (y/n)?
n

Enter endpoint 1 ( X(C1)  -T(K)    ) coordinates:
0.6 1853

Enter endpoint 2 ( X(C1)  -T(K)    ) coordinates:
0.6 1493

How many points along the profile?
500

Select a property [enter 0 to finish]:
   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 or Wt%) of the system
7 - Mode (Vol, Mol, or Wt proportion) of a phase
8 - Composition (Mol 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)
25

Output cumulative modes (y/n)?
(see www.perplex.ethz.ch/perplex_options.html#cumulative_modes)
n

warning ver178 at T(K)= 1853. P(bar)= 2000. the shear modulus of: melt(HP) is missing or invalid and has been estimated from the default poisson ratio

warning ver178 at T(K)= 1767. P(bar)= 2000. the shear modulus of: Fsp(C1) is missing or invalid and has been estimated from the default poisson ratio

warning ver178 at T(K)= 1766. P(bar)= 2000. the shear modulus of: melt(HP) is missing or invalid and has been estimated from the default poisson ratio

warning ver178 at T(K)= 1766. P(bar)= 2000. the shear modulus of: Fsp(C1) is missing or invalid and has been estimated from the default poisson ratio

warning ver178 at T(K)= 1766. P(bar)= 2000. the shear modulus of: melt(HP) is missing or invalid and has been estimated from the default poisson ratio

warning ver178 at T(K)= 1766. P(bar)= 2000. the shear modulus of: Fsp(C1) is missing or invalid and has been estimated from the default poisson ratio

warning ver178 at T(K)= 1765. P(bar)= 2000. the shear modulus of: melt(HP) is missing or invalid and has been estimated from the default poisson ratio

warning ver178 at T(K)= 1765. P(bar)= 2000. the shear modulus of: Fsp(C1) is missing or invalid and has been estimated from the default poisson ratio

warning ver178 at T(K)= 1764. P(bar)= 2000. the shear modulus of: melt(HP) is missing or invalid and has been estimated from the default poisson ratio

warning ver178 at T(K)= 1764. P(bar)= 2000. the shear modulus of: Fsp(C1) is missing or invalid and has been estimated from the default poisson ratio

warning ver178 at T(K)= 1764. P(bar)= 2000. the shear modulus of: melt(HP) is missing or invalid and has been estimated from the default poisson ratio

warning ver049 warning 178 will not be repeated for future instances of this problem. currently in routine: GETPHP

Data ranges excluding values equal to bad_number (NaN) specified in perplex_option.dat:

	abh	melt(HP)	Fsp(C1)	Fsp(C1)
min	0.000000	0.000000	0.000000	0.000000
max	0.000000	100.0000	100.0000	0.000000

Output has been written to two files:

plt format is in file: ab_an_melt_4.plt
1d tab format is in file: ab_an_melt_4.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:
www.perplex.ethz.ch/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
3

Construct a non-linear profile (y/n)?
n

Enter endpoint 1 (X(C1) -T(K)) coordinates:
0.6 1853

Enter endpoint 2 (X(C1) -T(K)) coordinates:
0.6 1493

How many points along the profile?
500

Select a property [enter 0 to finish]:
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 or Wt%) of the system
7 - Mode (Vol, Mol, or Wt proportion) of a phase
8 - Composition (Mol 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)
8

Enter solution or compound name (left justified):
melt(HP)

Compositions are defined as a ratio of the form:
    Sum {w(i)*n(i), i = 1, c1} / Sum {w(i)*n(i), i = c2, c3}
          n(j) = mole proportion of component j
          w(j) = weighting factor of component j (usually 1)

How many components in the numerator of the composition (<13)?
1

Enter component indices and weighting factors for the numerator:
  1 - ab
  2 - an
2 1

How many components in the denominator of the composition (<12)?
Enter zero to use the numerator as a composition.
2

Enter component indices and weighting factors for the denominator:
  1 - ab
  2 - an
1 1
```

2 1

The compositional variable is:

1.0 an

divided by

1.0 ab + 1.0 an

Change it (y/n)?
n

This composition will be designated: C1melt(HP)

Select a property [enter 0 to finish]:
8

Enter solution or compound name (left justified):
Fsp(C1)

Compositions are defined as a ratio of the form:
Sum {w(i)*n(i), i = 1, c1} / Sum {w(i)*n(i), i = c2, c3}
n(j) = mole proportion of component j
w(j) = weighting factor of component j (usually 1)

How many components in the numerator of the composition (<13)?
1

Enter component indices and weighting factors for the numerator:
1 - ab
2 - an
2 1

How many components in the denominator of the composition (<12)?
Enter zero to use the numerator as a composition.
2

Enter component indices and weighting factors for the denominator:
1 - ab
2 - an
1 1
2 1

The compositional variable is:

1.0 an

divided by

1.0 ab + 1.0 an

Change it (y/n)?
n

This composition will be designated: C2Fsp(C1)

Select a property [enter 0 to finish]:
0

Data ranges excluding values equal to bad_number (NaN) specified in perplex_option.dat:

	C1melt(HP)	C2Fsp(C1)
min	0.000000	0.000000
max	0.6016949	100.0000

Output has been written to the 1d tab format file: ab_an_melt_5.tab

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:
www.perplex.ethz.ch/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

C:\Users\Terezka\Documents\Perple_X clear>