# GeoPS: an interactive visualization tool for thermodynamic modeling of phase equilibria

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**Abstract**

Due to the progress of the availability of thermodynamic data in the last decades, equilibrium thermodynamics provides the ability to calculate mineral stability relations in the Earth's lithosphere (and beyond) as well as thermobarometric results. GeoPS (available at http://www.geops.org) is a windows-based interactive visualization program for thermodynamic modeling of phase equilibria. This program provides a wide range of phase equilibrium calculations and illustration facilities base on Gibbs free energy minimization method, which is done automatically with practically no user intervention. Possible applications include calculation various types of phase diagrams, isopleths, and thermodynamic modeling of phase equilibrium along specific P-T path with a progressively changing effective bulk compositions (EBC), such as fluid and melt loss, and chemical fractionation during compositionally zoned minerals growth in a metamorphic process. A novel algorithm with parallel computing makes GeoPS have high efficiency. The easy to use interface, visualization, high efficiency, reliability of GeoPS makes phase equilibrium modeling accessible to any researchers and students of earth sciences, and provides a powerful tool to understand natural systems and plan experimental work.

# GeoPS: an interactive visualization tool for thermodynamic modeling of phase equilibria

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**Key Points:**

- Phase equilibria modeling can quantify metamorphic and magmatic processes
- GeoPS is an interactive visualization program for thermodynamic modeling of phase equilibria
- The easiness to use, high efficiency and reliability makes phase equilibrium modeling accessible to anyone in need.

**Abstract**

Due to the progress of the availability of thermodynamic data in the last decades, equilibrium thermodynamics provides the ability to calculate mineral stability relations in the Earth's lithosphere (and beyond) as well as thermobarometric results. GeoPS (available at http://www.geops.org) is a windows-based interactive visualization program for thermodynamic modeling of phase equilibria. This program provides a wide range of phase equilibrium calculations and illustration facilities base on Gibbs free energy minimization method, which is done automatically with practically no user intervention. Possible applications include calculation various types of phase diagrams, isopleths, and thermodynamic modeling of phase equilibrium along specific P-T path with a progressively changing effective bulk compositions (EBC), such as fluid and melt loss, and chemical fractionation during compositionally zoned minerals growth in a metamorphic process. A novel algorithm with parallel computing makes GeoPS have high efficiency. The easy to use interface, visualization, high efficiency, reliability of GeoPS makes phase equilibrium modeling accessible to any researchers and students of earth sciences, and provides a powerful tool to understand natural systems and plan experimental work.

**Keywords**: GeoPS, thermodynamic modeling, phase equilibrium, visual computing

## 1. Introduction

It is an important goal for petrologist to determine the formation and metamorphic conditions of rocks throughout Earth's history. Equilibrium thermodynamics, as the physical basis for developing geothermobarometric tools, is very powerful in petrology. Based on the fundamental principle of equilibrium thermodynamics, it has been recognized that the mineral assemblages and their composition of the rocks depend on temperature (T), pressure (P), and bulk composition ($X_{sys}$). Accurate thermodynamic modeling of natural rocks is a huge challenge and one of the most desirable tasks. In the last decades significant progress of thermodynamic dataset for phases of petrological interest has been made in the ability to predict complex assemblages, composition and phase relations (Ghiorso & Sack, 1995; Ghiorso et al., 2002; Holland & Powell, 1998, 2011; Holland et al., 2018; Stixrude & Lithgow-Bertelloni, 2011; White et al., 2014).

Phase equilibrium modeling has recently been considered the best way to extract P-T information from metamorphic rocks (Powell & Holland, 2010). At present, there are numerous computer programs for calculation of equilibrium phase diagrams (or pseudosection), each applying a different strategy. Among them, three are particularly prevalent among petrologists: THERMOCALC (Powell et al., 1998), Perple_X (Connolly, 1990; Connolly, 2005), Theriak/Domino (de Capitani & Brown, 1987; de Capitani & Petrakakis, 2010). Each program has its own advantages and limits that have been briefly summarized by Lanari and Duesterhoeft (2018). However, one of their common characteristics is the fact that they are console applications, not very user-friendly, especially for new or novice users.

In this contribution we present a windows-based interactive program named GeoPS that is a visual computing platform for phase equilibrium modeling base on Gibbs free energy minimization method. GeoPS provide a wide range of phase equilibrium calculations and illustration facilities. GeoPS can be used to compute equilibrium assemblages, chemical and physical properties of phases along given P-T-$X_{sys}$ path or grid and generate various kinds of diagram. Its powerful function, easy operation high efficiency and reliability makes it accessible not only to a few specialists, but also practically to anyone in need. Although a beta test version has been released for some time, it has only recently reached some state of robustness and fully function. Here we present instructions and some illustrative examples that highlight the main advantages of GeoPS.

## 2. Strategy of GeoPS

There are two generic methods in different programs to generate phase diagrams: phase equilibrium calculators (e.g., THERMOCALC by Powell et al. 1998) and Gibbs free energy minimizers (e.g., Perple_X by Connolly 1990; THERIAK-DOMINO by de Capitani & Brown, 1987). Each method has its own advantages and limits that have been briefly summarized by Connolly (2017). Connolly (2017) have briefly summarized the advantages and limits of each method. The THERMOCALC algorithm is to compute the compositions of the phases for a specified phase assemblage which requires to be judged and thus strongly relies on the expertise of the user (Connolly, 2017; Lanari & Duesterhoeft, 2018). In contrast, Gibbs free energy minimizers consider all of the phases present in a given thermodynamic dataset, which method is used in GeoPS as well as Perple_X and THERIAK-DOMINO. GeoPS determines the equilibrium assemblages and

properties for given P-T-$X_{sys}$ points rather than the position of field boundaries. And then the multidimensional P-T-$X_{sys}$ phase diagram of a thermodynamic system can be mapped by Gibbs free energy minimization. An efficient parallel algorithm is used to accelerate mapping on multicore platforms.

## 2.1. The algorithm of Gibbs free energy minimization

In GeoPS, the Gibbs free energy of the system is expressed as function of the Gibbs free energies of its constituent phases:

$$G^{sys} = \sum_{j=1}^{p} \alpha_j \, G_j \qquad (1)$$

where $\alpha_j$ , $G_j$ are the molar amount and Gibbs energy of species j, respectively. And p is the total number of constituent phases in the system. Mass balance further requires that the sum of quantities of the components in each phase of the system must equal the corresponding quantities in the system, i.e.

$$X_i^{sys} = \sum_{i=1}^{c} \alpha_j \, x_{ij} \qquad (2)$$

where c is the number of components, and $x_{ij}$ is the quantity of the component i in the phase j.

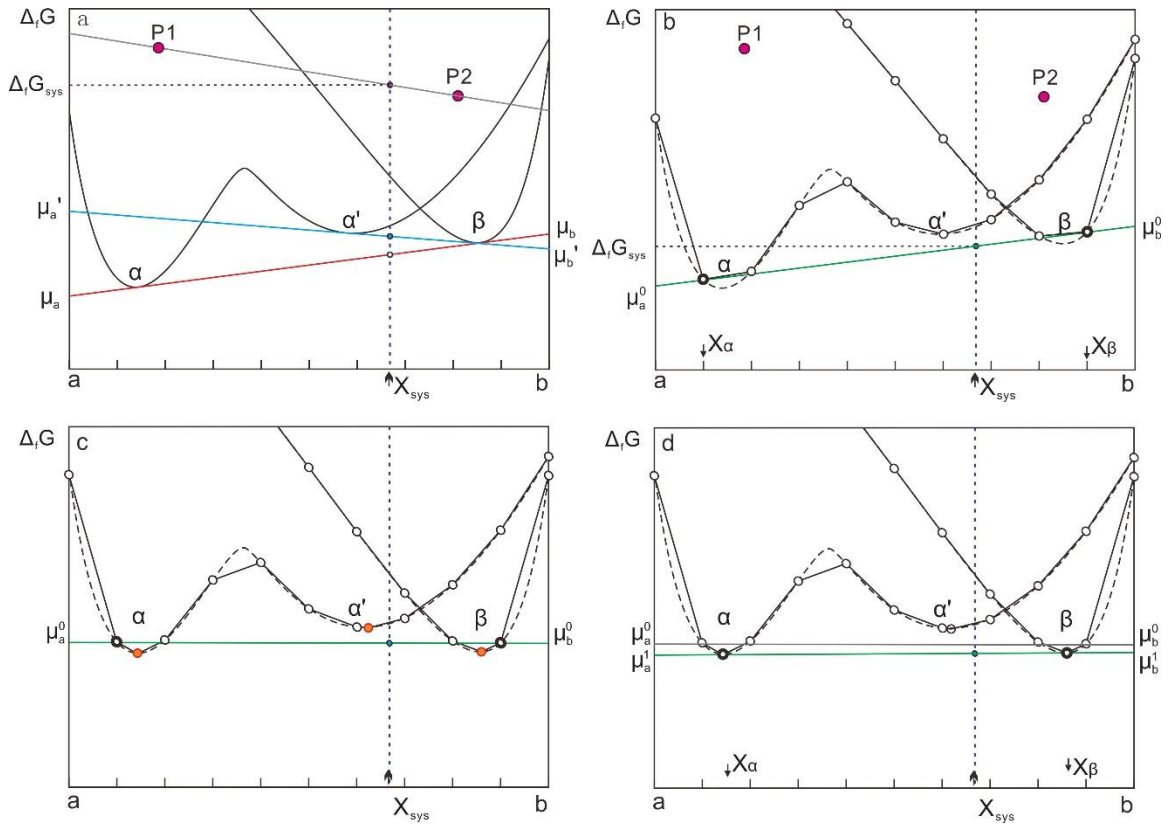



Fig. 1. Schematic illustration of the GeoPS algorithm for a binary (c = 2), isobaric-isothermal, system with composition $X_{sys}$. (a) All possible states of matter are described by two solution phases (dashed curves) and two pure phases (filled circles). (b) Each equation of state of the solution phase is represented by a finite set of points (circular symbols). The initial solution (filled circles in b) is obtained by linear programming. This solution defines a g-x plane and chemical potentials $\mu_a^0$ and $\mu_b^0$. (c) Given these chemical potentials the g-coordinates of and are transformed according to Eq. (4); The minima in the transformed functions and are then located by non-linear programming. (d) A new solution (filled circles in d) is obtained from these minima and the previous solution by linear programming (filled circles in b, gray circles indicate the previous solution). These steps are repeated iteratively until the phase compositions converge within the desired tolerance.

The Gibbs free energy minimization problem is to determine the quantity and compositions of the phases that minimize the $G^{sys}$ at constant P-T-$X_{sys}$. Gibbs free energy minimization is a simple linearization problem while the system consists of only pure

phases. However, if solution phases are involved the problem becomes non-linear (Connolly, 2005). Consequently, it is complicated to exactly solve the phase equilibrium problems which is necessary to refine the stable phases and its compositions by iteration (non-linear programming). On the other way, the continuous solid solutions can be approximated by a finite number of discrete phase states (pseudo-compounds), and then the phase equilibrium problem reduces to a linear optimization problem that can be solved by linear programming (Connolly, 2005).

Both linear and Non-linear Gibbs energy minimization strategies are used in available software packages. Each strategy has its own advantages and limits Connolly (2017). Non-linear Gibbs free energy minimization strategies might converge to local minima (Connolly, 2017). However, the limitations of linear Gibbs energy minimization are that it becomes inefficient with the large numbers of pseudo-compounds necessary to represent accurately the composition of complex solutions (i.e. amphibolite, biotite, silicate melts) (Connolly, 2005).

In this paper, we propose hybrid Gibbs free energy minimization algorithm which aims at combining the strengths of both linear and non-linear scheme. GeoPS applies a series of linear and non-linear programming steps (Fig. 1).

Firstly, linearized Gibbs energy minimization are utilized to derive the initial solution. A finite number of pseudo-compounds are used to approximate the continuous states of solution with relatively low compositional resolution. In the approximated system, the Gibbs energy minimization problem becomes a linear optimization problem, and the initial results can be solved by linear programming.

Secondly, refining the compositions of the potential stable phases by iteration to get

accurate solutions. This initial solution defines the g-x plane (Fig. 1b)

$$g = \sum_{i=1}^{c} x_i \mu_i \quad (3)$$

The complete set of $g'_j(x)$ functions of interest are then transformed as

$$g'_j(x) = G_j(x) - g(x) \quad (4)$$

Then, the minima of the individual $g'_j(x)$ functions are located by a gradient descent method. There is a risk of that a low-resolution Linearized Gibbs energy minimization may not identify the phases that would be stable at higher resolution. To avoid this risk, it is essential to locate the minima of $g'(x)$ of the metastable solution phases, which are close to the g-x plane of the previous solution, as well as those that are stable. The new pseudo-compounds with minima of $g'(x)$ are added into the list of pseudo-compounds. And then the linear programming step is repeated considering these minima and the phases of the initial solution. These steps are repeated iteratively until the solution is judged to have converged to the global minimum.

### 2.2. A strategy of adaptive refinement of triangular meshes for mapping phase diagram sections

GeoPS compute stable mineral assemblages for specific P–T–Xsys points (i.e. within stability fields) base on Gibbs free energy minimization. The stability fields of each assemblages are determined by grid mapping. The phase diagrams are produced through outline the stability fields with interpolation between stability fields. Furthermore, a multilevel grid strategy is needed to reduce the number of minimizations and improve efficiency as well (e.g. Connolly, 2005; de Capitani & Petrakakis, 2010).

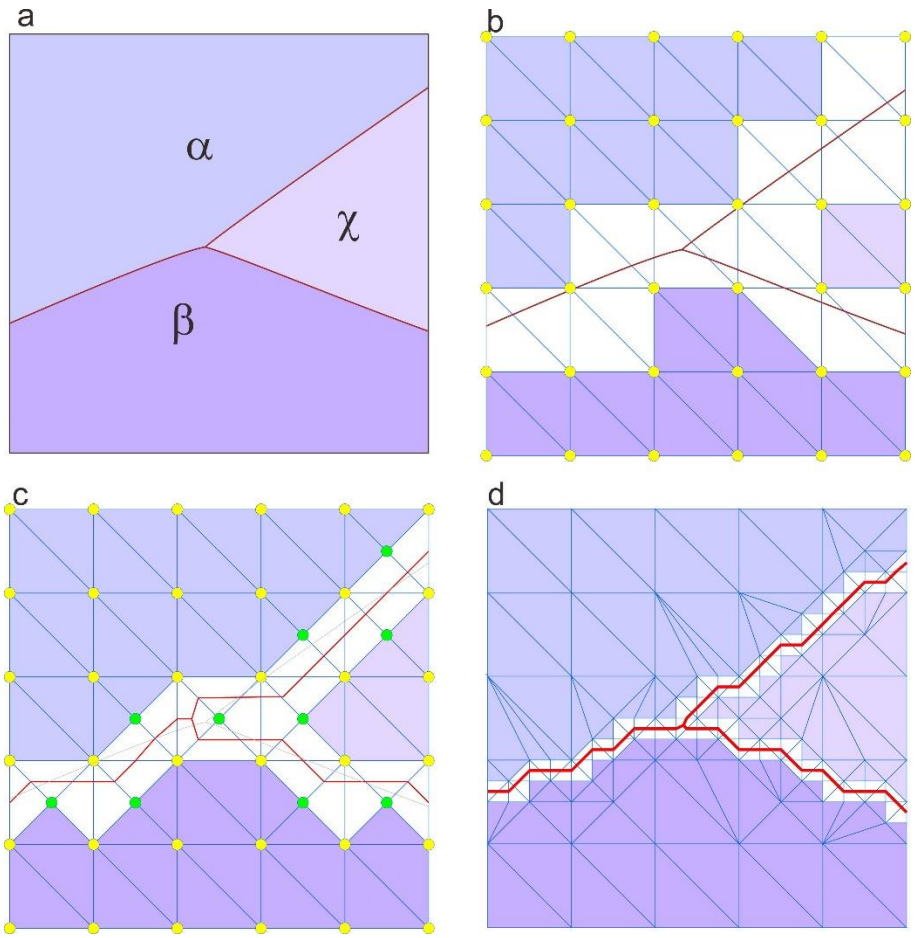



Fig. 2. Sketch of the GeoPS algorithm. See text for details. (a) Sample diagram with definition of initial grid. (b) determining Stable assemblages of each notes in the initial grid, and identifying which triangles need refinement. (c) Refining the marked triangles, determining stable assemblages of new notes, and identifying which triangles need refinement. These steps are repeated iteratively until the effective resolution reached the requirement. (d) shows the result after 4 steps are repeated.

In GeoPS, an unstructured triangular grid that supports local adaptive mesh refinement is adopted. Firstly, the xy-space is divided into triangular with a regular grid which has $N_x$ and $N_y$ sampling points on the horizontal and vertical axes (Fig.2b). The equilibrium assemblage of each grid node is calculated by Gibbs free energy minimizer. If the same mineral assemblage is stable at three nodes of a triangle, then the mineral

assemblage is assumed to be stable in the triangle. Likewise, heterogeneous triangles are marked for investigation in the next step. Each of these marked triangles is divided into two triangles, through adding a new node on the midpoint of the long side. At the same time, the neighboring triangle also is divided into two triangles. The stable mineral assemblage at each of the new nodes are predicted by free energy minimizer, and heterogeneous triangles are again marked for investigation. These steps are repeated until the effective resolution, which is defined by the length of the long side of the triangle, reached the requirement (Fig. 2c).

## 3. Description of the program

GeoPS is a visual computing platform for thermodynamic modeling of phase equilibrium. The soft can run on Windows with the .NET Framework 4.5 or later versions. The source code is written in MS Visual Basic.Net. The software and the tutorial are available online at http://www.geops.org.

GeoPS provides a series of functions for thermodynamic equilibrium calculations and illustration facilities. And more functions will be extended with future development. This program includes a set of user-friendly graphical user interfaces for the different steps of the procedure. The main interface of GeoPS shows in Fig.3. The other function windows can be open through the menus on the main interface.

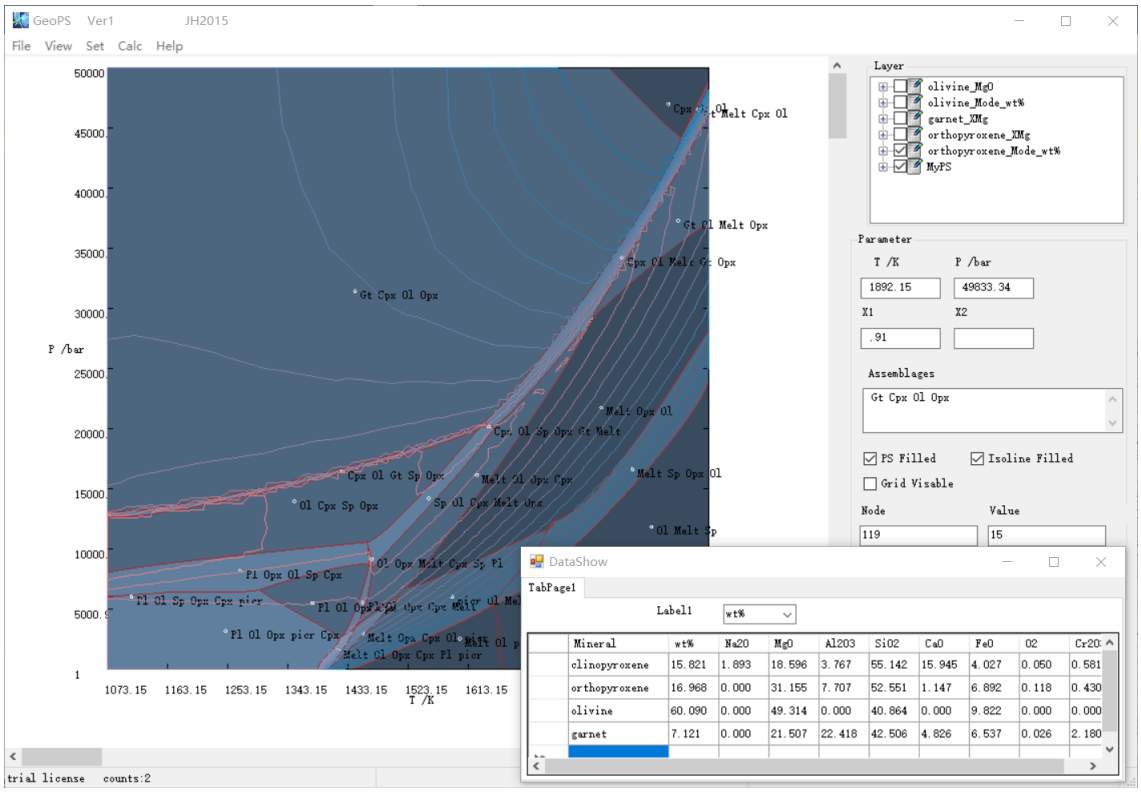
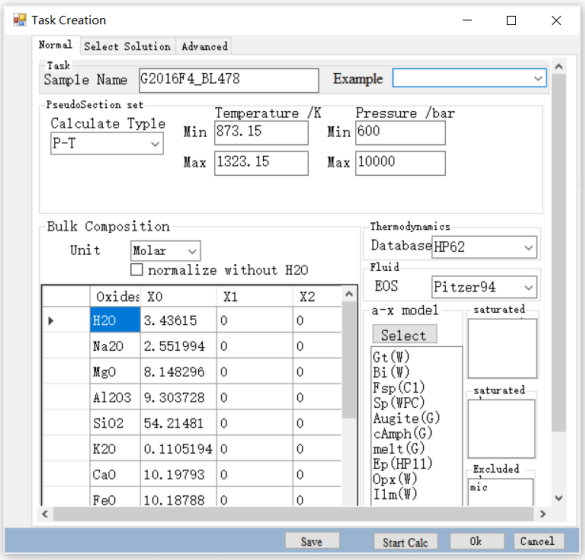



Fig. 3, The screenshot of main interface of GeoPS. The displayed image is a P–T pseudosection and isopleths of modal of Opx calculated for KLB-1 in the NCFMASOCr system, which bulk compositions is same with the Fig. 1 of (Jennings and Holland, 2015). In the lower right is the "DataShow" window which can show the result data of the point of mouse click in the pseudosection.

### 3.1. Creating task and calculating

In the task creation window (Fig.4), the user can open and modify an exist task as well as create a new one. For calculating P-T pseudosections, it is only necessary to set the bulk composition and P-T range. Additionally, users also are allowed to change the calculation type, the version of the internally consistent thermodynamic dataset and mineral activity models. There are several types of calculation can be selected (Table 1). For the bulk composition, user can enter weight percentage or mole percentage. The soft will automatically convert the composition into mole percentage and normalize.




199

200 Fig. 4. an example screenshot of a task creation window.

201

202 Table 1. The types of phase equilibrium calculation in GeoPS

| Index | Type | Description | P-T setting | Bulk setting |
|---|---|---|---|---|
| 1 | Line | Equilibria calculated along the P-T path | P=P0+(P1-P0)*i/N<br>T=T0+(T1-T0)*i/N<br>N is steps, i=0 to N | Only X0 is required |
| 2 | P-T | P-T psudosection，x-axes is temperature，Y-axes is pressure | P=P0+(P1-P0)*y, 0≤y≤1<br>T=T0+(T1-T0)*x, 0≤x≤1 | Only X0 is required |
| 3 | P-X | P-X psudosection，x-axes is the proportion of X1，Y-axes is pressure | P=P0+(P1-P0)*y,<br>T=T0+(T1-T0)*y, 0≤y≤1<br>P1>P0; While T0=T1, means T is fixed | X0 and X1 are required |
| 4 | T-X | T-X psudosection，X-axes is the proportion of X1，Y-axes is temperature | P=P0+(P1-P0)*y, 0≤y≤1<br>T=T0+(T1-T0)*y,<br>T1>T0; while P1=P0, means P is fixed | X0 and X1 are required |
| 5 | X-X | X-X psudosection，X-axes is the proportion of X1，Y-axes is the proportion of X2 | Specific P and T<br>T=T0<br>P=P0 | X0, X1 and X2 are required |

203

204 And then, click the button of “Start Calc”, the soft will start computing automatically.

205 The initial phase diagram will be displayed on the main interface after a few seconds to

206 minutes, which depend on the complexity of the considered solutions. And the phase

diagram will be refined continually until the effective resolution reached the requirement (Fig. 5).

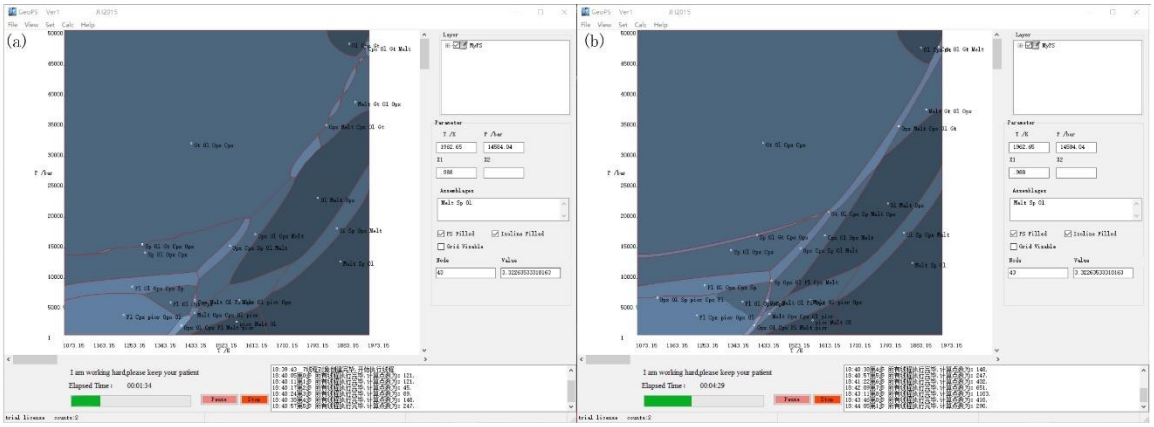



Fig. 5. Screenshots of different time during calculating P-T pseudosection for KLB-1 in the NCFMASOCr system. (a) and (b) are the screenshot after 1.5 and 4.5 minutes of running time, respectively. The example was calculated on a laptop with a 2.60GHz Inter® Core™ i7-6700HQ CPU and 16GB of RAM, Microsoft Windows 10 Home x64 operating system.

### 3.2. Showing results and calculating isopleths

The phase diagram of the different stage during calculating will be displayed on the main interface, and the user is allowed to use the "DataShow" window to view the result data of the point of the mouse click in the phase diagram (Fig.3). The results of each point include the P-T, mineral assemblage, modal and composition of each phase, etc.

The Isopleth calculation window can be open while the phase diagram calculation has been finished. In the Isopleth calculation window, the user needs to select the mineral phase and its property. The user can select pre-programmed property (e.g. modal abundance, composition, molar volume, density, etc.) as well as enter a formula to custom property. The soft will automatically give the range of values and interval of isolines which also are allowed to change. Then click the OK button, the isopleth will be

displayed on the main interface in a few seconds. GeoPS also allows the user to modify the start/end value and interval, contour color and fill color of the isopleths through double click on the layer from the Layer panel.

### 3.3. Output results

GeoPS can output the pseudosection and isopleths in a range of useful image formats, including the Scalable Vector Graphics (SVG) format and bitmap formats, such as JPEG and BMP. The calculated results, including assemblages, mode and compositions of phases, etc., can output in CSV format which can be analyzed directly in excel.

## 4. Tests and evaluation

In order to assess the validity of GeoPS, sample BL478 from Green et al. (2016) will be repeatedly used in the following. The P-T and T-X Pseudo-sections of this sample were published in Green et al. (2016). The database used here is versions 6.2 of Holland and Powell (2011) with improved solution models for white mica, biotite, garnet, chlorite, orthopyroxene is from White et al. (2014), Amphibole, clinopyroxene, melt is from Green et al. (2016), feldspar is from Holland and Powell (2003). The bulk composition in moles of BL478 is SiO2 (53.96), TiO2 (1.35), Al2O3 (9.26), FeO (10.14), MgO (8.11), Ca (10.15), Na2O (2.54), K2O (0.11), and O2 (0.49), H2O (3.42), which is from the table 1 of Green et al. (2016).

### 4.1. Calculate equilibrium phase diagrams

Calculation equilibrium phase diagram is useful to constrain the P-T conditions for the observed mineral assemblages in natural rocks. This diagram also can help to understand mineral evolution during the metamorphism. The program GeoPS can various kinds of phase diagram, and also can provide detailed information about contents and

compositions of phases in an equilibrium assemblage at any pressure and temperature in the diagram (Fig. 3). In order to demonstrate the reliability of GeoPS, the P-T pseudosections of sample BL478 is calculated by GeoPS and THERMOCALC (Powell et al., 1998) respectively with the same thermodynamic parameters. The phase diagram generated by GeoPS (Fig. 6b) is almost identical to that generated by THERMOCALC (Fig. 6a), and also is consistent with the Fig. 4a in Green et al. (2016).

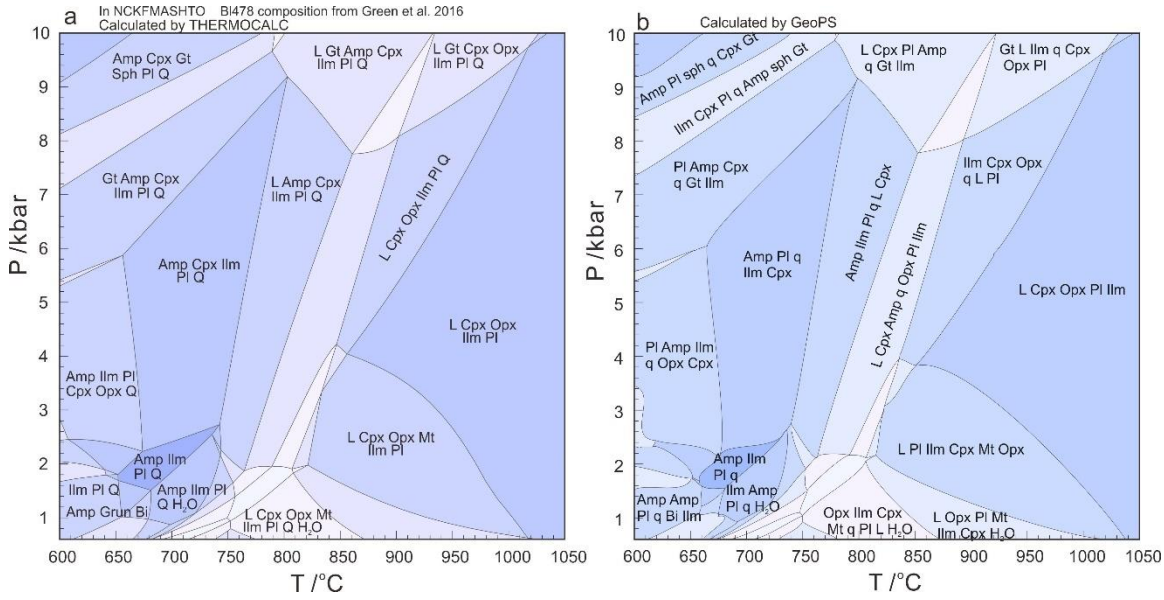



Fig 6. P–T pseudosections of sample BL478 which bulk composition is from Green et al. (2016). (a) calculated by THERMOCALC; (b) calculated by GeoPS.

To investigate the effect of system component variations on the stable assemblages, it is possible to calculate T-X or P-X pseudosections with GeoPS. Figure 7 for example, is a T-$X_{H2O}$ diagram which shows the effect of the $H_2O$ content on the stable assemblages in sample BL478. Two pseudo-binary end-member compositions are same with sample BL478 except the H2O content is 0 and 5 moles, respectively. This figure is consistent with the Fig. 4a in Green et al. (2016), which is calculated by THERMOCALC, except in

the left lower corner. In Fig. 6, a little bit biotite or k-feldspar are stable at the low temperature and low $H_2O$ content field. Probably the reason for this difference is that the biotite an k-feldspar are not considered during the calculation of the Fig. 4a in Green et al. (2016).

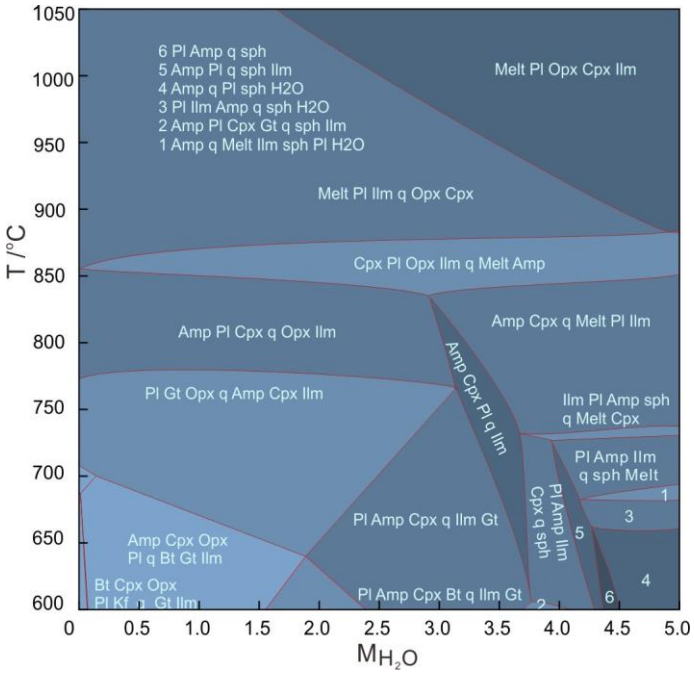



Fig 7. GeoPS calculated T–$M_{H2O}$ sections of sample BL478 at 7 kbar.

## 4.2. Calculate Isopleth

In a pseudosection of a given bulk composition, the predicted mineral assemblages can be compared with the natural record of a metamorphic rock. The P-T conditions for the observed mineral assemblages can be constrained in the P–T space of computed stability field. In order to further refine the P–T conditions and discussion on mineral evolution, it is required comparison of observed and predicted amount and compositions of minerals. For that purpose, isopleths of amount and/or compositions of phases can be

computed by GeoPS conveniently. As an example, the $X_{An}$ of plagioclase and the modal amount of melt expressed as vol% of solids is shown in Figure 8.

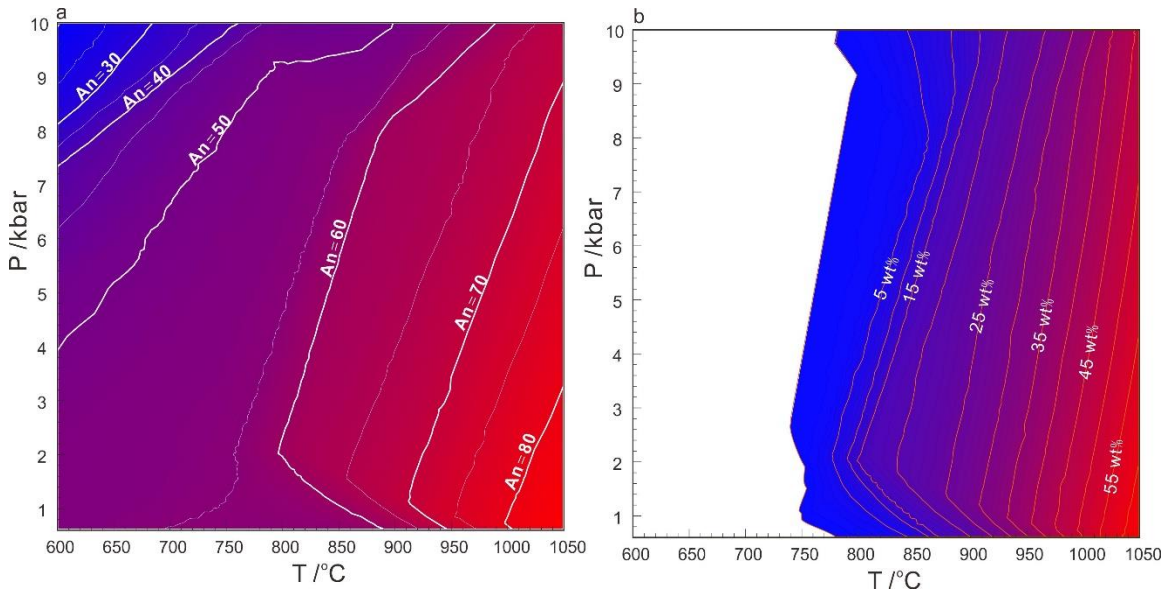



Fig. 8. Examples of isopleths computed by GeoPS using the composition of sample BL478. (a) isopleth of $X_{An}$ of plagioclase; (b) isopleth of melt mode.

### 4.3. Phase equilibrium modeling along a given P-T path

GeoPS also can be used to calculate phase equilibrium along a given P-T path to investigate the variations of mineral properties during the metamorphism. Effective bulk composition (EBC) of the system can be altered throughout the metamorphic process, such as, metamorphic dehydration and the volatile components escaping from the rocks on prograde segments, melt loss during anatectic process (Mayne et al., 2016; Spear & Wolfe, 2018). Thus, EBC of a system is dependent on the P–T path. The popular phase equilibrium modeling softs are inconvenient to handle the EBC changing dependent on the P–T path, despite there are several add-ons and extensions can be used for the simulation of melt loss and garnet growth (e.g. Gaidies et al., 2008; Mayne et al., 2016).

296 Using GeoPS, it is conveniently to calculate phase equilibrium along a given P-T path,
297 and allows altering the EBC of the system through phase additions or extractions
298 dependent on P-T trajectory.

299 To show the advanced functionality of GeoPS, a hypothetical clockwise P–T path is
300 investigated with the same starting bulk composition of Fig 6. The clockwise P–T path
301 (Fig. 9a) starts off with the heating from 600 °C, 6 kbar to 1000 °C, 10 kbar. This is
302 followed by an isothermal decompression to 1000 °C, 5.5 kbar and retrograde cooling
303 until 600 °C, 4 kbar. In order to investigate the effects of melt loss in an open system for
304 sample BL478, we calculated phase equilibrium along the P-T path with equilibrium
305 model and fractionation model, respectively. For the equilibrium model (Fig.9b), for each
306 step complete equilibrium, and EBC invariant is assumed. For the fractionation model
307 (Fig. 9c), EBC of the relative systems will change along the dependent path. Melt loss
308 was set to occur when a 7 wt.% threshold of melt was exceeded, and extraction left 1 wt.%
309 melt. It is assumed that the free $H_2O$ from metamorphic dehydration will escape from the
310 system immediately.

311 At the points B and C, compared with the closed system, the open system has a
312 significantly lower proportion of the cumulative total melt, higher proportion of
313 plagioclase. In the open system, because melt loss cumulatively depletes residuum H2O,
314 the granulite facies mineral assemblage of Opx+Cpx+Pl are retained during retrograde
315 cooling (Fig 9c). Besides the obvious differences in mineral assemblage and content
316 between the open system and the closed system, there are also obvious differences in
317 mineral composition (Fig 9d).

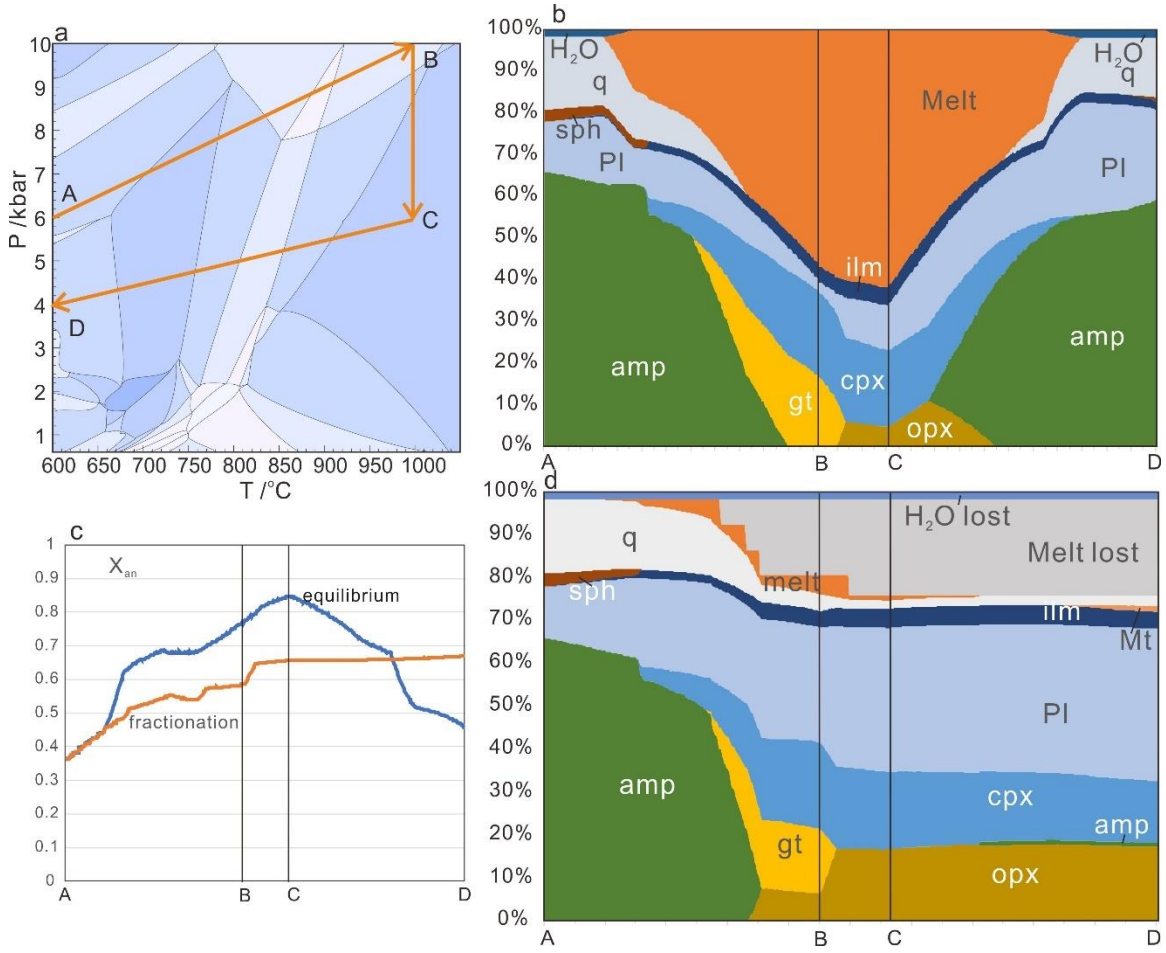



Fig 9. GeoPS calculated P–T pseudosection for the Sample BL478 with a hypothetical clockwise P–T path consisting of a prograde heating segment from 660 °C, 12 kbar to 950 °C, 10 kbar, followed by isothermal decompression to 950 °C, 5.5 kbar and retrograde cooling until 600 °C, 4 kbar. (b-c) Phase proportions along the clockwise P–T path for: (b) the closed system; (c) the open system. (d) Xan of plagioclase along the clockwise P-T path.

## 5. Conclusions

We describe the program GeoPS, a user-friendly, standalone Windows software which functions as an interactive visual computing system for the thermodynamic phase equilibrium. This soft is powerful in thermodynamic equilibrium calculations and illustration base on Gibbs free energy minimization method, which is done automatically

with practically no user intervention. The applications not only include calculation various pseudosections, isopleths, but also thermodynamically modeling of phase equilibrium along pre-defined P-T path with a progressively changing EBC. If the same thermodynamic dataset and solution models are used, the results are consistent with that calculated by THERMOCALC. The visualization, high efficiency and friendly interactive interface makes thermodynamic phase equilibrium modeling accessible to any researchers and students of earth sciences, and provides a powerful tool to understand natural systems and plan experimental work.

**Acknowledgements**

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