Journal of Sciences, Islamic Republic of Iran 22(4): 345-349 (2011) http://jsciences.ut.ac.ir
University of Tehran, ISSN 1016-1104

APG: An Efficient Software Program for Amp-Pl Thermobarometry Based on Graphical Method

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Received: 17 September 2011 / Revised: 27 December 2011 / Accepted: 9 January 2012

Abstract

Geothermobarometry equations are based on thermodynamic principles and appear in single or multi-variant functions. The number of variants for a specific composition or reaction usually is reduced into 2 involving temperature (T) and pressure (P). Since most of planned equations have two passive or variant P and T, using these equations should be with special care. It is very effective to use graphical method to apply geothermobarometry functions. Graphical method is a fundamental way to solve the math functions. In the graphical method two consistent geothermobarometry equations, which both have at least one share variant (P or T), are selected in order to achieve P and T. These selected equations should be applicable for the same reaction or rock. In this method selected thermobarometry equations are drawn on a P-T diagram and then intersection point of them which introduces asked temperature and pressure will be obtained. One of the most common geothermobarometry equations, suitable for intermediate magmatic rocks, is amphibole-plagioclase thermometry and amphibole barometry. APG software program introduced in this paper is specialized and designed for calculating equilibrium temperature and pressure of amphibole and plagioclase within an igneous rock. In this software program, Pressure and temperature are estimated coincidently based on the graphical method.

Keywords: APG software program; Amphibole; Plagioclase; Graphical method; Geothermobarometry

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Introduction

It is very important for petrologists to estimate physical conditions prevailed during petrological processes such as temperature and pressure of crystallization of a certain phase from a magma or temperature and pressure of equilibrium through metamorphic reactions. In the petrology of rocks, geothermobarometry equations are used to determine temperature and pressure [15, 18, 21]. One of the most common geothermobarometry equations suitable for intermediate magmatic rocks is amphibole-plagioclase thermometry (Amp-Pl thermometry) and amphibole barometry. Since amphibole and plagioclase exist

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compatibly not only in most intermediate igneous rocks but also in some of acidic and basic igneous rocks, using Amp-Pl geothermobarometry has become an effective tool for estimating physical conditions of crystallization of amphibole and plagioclase, and physical conditions of magma-cooling. Although there are several software programs based on amphibole barometry and Amp-Pl thermometry, but in none of them calculating of temperature and pressure is done coincidently. This defect can lead to calculating errors and ambiguity. Therefore, the lack of an efficient visual software program based on drawing of math functions is obvious. The aim of this paper is to introduce a new software program based on graphical method for deriving temperature and pressure from equations of Amp-Pl thermometer and amphibole barometer.

Materials and Methods

Basically, a geothermobarometry equation is a function between pressure (P) and temperature (T) which introduces a line or a curve on the P-T diagram. Geothermobarometry equations are divided into two types. One is geothermometry and the other is geobarometry. Geothermometers (geothermometry equations) have low value of $\frac{dP}{dT}$ when they are displayed on the P-T diagram. In other words, geothermometers are very sensitive to temperature variations, but they are hardly dependent on pressure. On the other hand, geobarometers are characterized by having high value of $\frac{dP}{dT}$ when they are drawn on the P-T diagram. That means they are much more sensitive to pressure variations rather than temperature variations (Fig. 1).

Most of the suggested calibrations of geothermobarometers in petrology involve two variants of T and P for example: amphibole-plagioclase thermometry [6], amphibole barometry [1], single clinopyroxene geothermobarometry [14], garnet-clinopyroxene geothermometry [4,9,10,12,13,16,17]. To use these equations to estimate P and T, it must be noticed that by assuming constant values for each of variants (P or T) and inputting in the equation, the actual answer can not be derived. This way has some defects outlined as the following:

1. Considering a range of P and inputting in the geothermometer equation to determine T can cause missing actual range of P and also wrong answer for T. This state is also occurred for estimating P by using a geobarometer when T is supposed in an assumed range. Uncertainty of this defect is heavily depended on the dip of used function (geothermobarometry equation).

2. Considering a wide range of pressure and temperature. In the example above, if pressure is supposed in the range of 1-20 kbar and on the base of this pressure range, therefore, there would be a wide range of P and T only for one mineral. Whereas, a geothermobarometer for a mineral introduces only one point of P and T plus a known uncertainty which is an invariant point.

Since this way calculates a range of T and P, it will be very difficult or impossible to interpret for several minerals that crystallized in different conditions of P and T.

Results and Discusion

Graphical Method

Graphical method is a fundamental way to solve the math functions. In this way a couple of geothermobarometry equations required to be drawn on the P-T diagram. These equations are almost two-variant P-T dependent equations.

When two equations were plotted on the P-T diagram, the asked P and T are easily obtained from the intersection point of the two equations. The highly important point in using graphical method for calculating P and T is selecting two suitable equations. Appointing to the kind of rock and geothermobarometer presented for, limitation using affirmed by presenter is very essential in selection of equations unless output answers are invalid. Advantages of graphical method can be outlined as: (1) Having been drawn, geothermobarometry equations show how their circumstances are. (2) Range of description can be selected according to beneficial purpose and accuracy. (3) Some of the factors in geothermobarometry equations which are dependent on P or T are computed in a constant value by some softwares, but in the graphical method their thermal or pressure depending can be applied in the equation.

APG Software Program

This software is a completely user friendly program that is being introduced for the first time. This software program is designed for estimating equilibrium temperature and pressure of amphibole and plagioclase within an igneous rock. In this software, pressure and temperature are calculated coincidently based on the graphical method. Layout of this software program is exhibited in Figure 2. Amphibole parameters (inputs in the Amp panel) must be in a.p.f.u. (atom per formula

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unit). Ab and An (inputs in the Plg panel) are Values of albite and anorthite content respectively in the plagioclase normalized to 0 to 1.

Required inputs can be easily gained from structural formula of amphiboles [6, 11] and feldspars [3] which are resulted from a microprobe analysis of a pair Amp-Pl in equilibrium in a magmatic rock. Although method presented by Leake [11] is prevalent and newer than Holland and Blundy [6], to calculate the structural formula of amphiboles, it is recommended to use Holland and Blundy method [6] because calibrations of thermometers were based on this method.

In order to plot barometer equation curve, five calibrations are regarded that can be easily selected from the barometer popup menu of APG. These calibrations are listed as equations 1 through 5.

1) $P(\pm 3kbar) = -3.92 + 5.03Al_{total}$, [5]

2) $P(\pm 1kbar) = -4.76 + 5.64Al_{total}$, [7]

3) $P(\pm 1kbar) = -3.46 + 4.23Al_{total}$, [8]

4) $P(\pm 0.6kbar) = -3.01 + 4.76Al_{total}$, [20]

5) $P(\pm 0.6kbar) = 4.76Al - 3.01 - [(\frac{T(℃) - 675}{85}) \times (0.53Al + 0.005294 \times (T(℃) - 675))]$, [1]

In order to draw thermometer equation curve, 3 calibrations are available which two of them (equations 6 and 7) are introduced by Holland and Blundy [6] and the other (equation8) is presented by Blundy and Holland [2]. These calibrations, shown as equations 6, 7 and 8, are settled in the thermometer popup menu of APG and easily can be selected.

6) $$T(\pm 40℃) = \frac{-76.95 + 0.79P + Y_{ab} + 39.4X_{Na}^{A} + 22.4X_{K}^{A} + (41.5 - 2.89P)X_{Al}^{M2}}{-0.0650 - 0.0083144Ln\left(\frac{27X_{vac}^{A}X_{Si}^{T1}X_{ab}^{pl}}{256X_{Na}^{A}X_{Al}^{T}}\right)} - 273.15$$

Y_{ab} =0 for X_{ab}^{pl} > 0.5 or else $Y_{ab} = 12\left(1 - X_{ab}^{pl}\right)^2 - 3kj$

7) $$T(\pm 40 \circ C) = \frac{78.44 - Y_{ab-an} - 33.6X_{Na}^{M4} - (66.8 - 2.92P).X_{Al}^{M2} + 78.5X_{Al}^{T1} + 9.4X_{Na}^{A}}{0.0721 - 0.0083144Ln\left(\frac{27.X_{Na}^{M4}.X_{Si}^{T1}.X_{an}^{pl}}{64.X_{Ca}^{M4}.X_{Al}^{T1}.X_{ab}^{pl}}\right)} - 273.15$$

Y_{ab-an} = 3 kj for X_{ab}^{pl} >0.5 or else $Y_{ab-an} = 12\left(2.X_{ab}^{pl} - 1\right) + 3kj$

8) $$T(\pm 40 \circ C) = \frac{0.677P - 48.98}{-0.0429 - 0.0083144Ln\left(\left[\frac{Si - 4}{8 - Si}\right].X_{ab}^{pl}\right)}$$

where T is expressed in °C, X terms (molar fractions) are defined in [6] which are outlined as

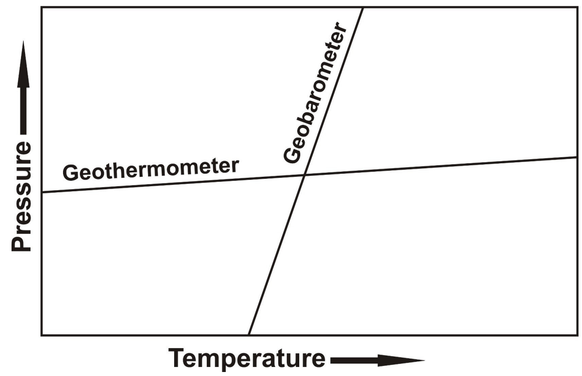

Figure 1. Diagram of P versus T (P-T diagram). Geothermometer and geobarometer are shown (notice to dips of them).

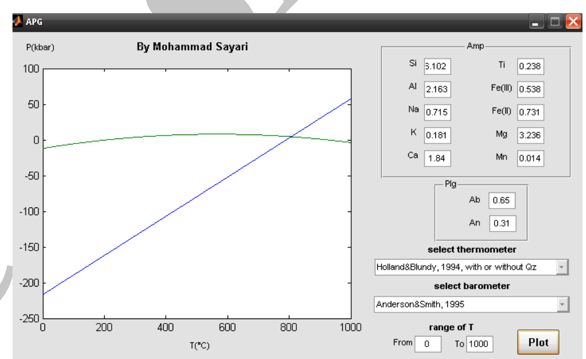

Figure 2. Layout of APG software program.

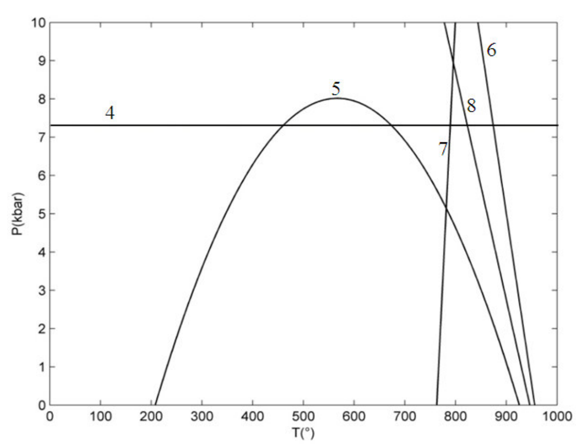

Figure 3. Exhibiting equations 4-8 for a pair coexisting Amp-Pl in an andesite [19].

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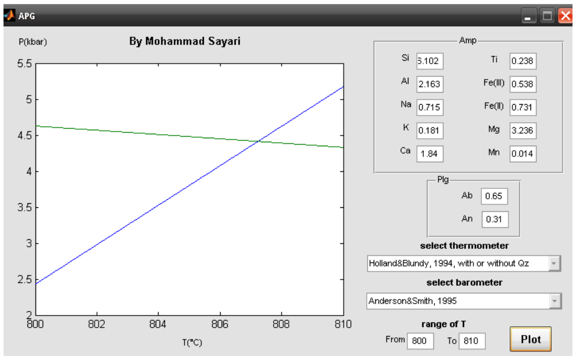

Figure 4. The temperature data range is limited to 800-810°C.

$X_{Si}^{T1} = (Si - 4)/4$
$X_{Al}^{T1} = (8-Si)/4$
$X_{Al}^{M2} = (Al + Si - 8)/2$
$X_{K}^{A} = K$
$X_{v}^{A} = 3-Ca-Na-K-cm$
$X_{Na}^{A} = Ca+Na+cm-2$
$X_{Na}^{M4} = (2 - Ca- cm)/2$
$X_{Ca}^{M4} = Ca/2$
$cm = Si+Al+ Ti+ Fe^{3+} + Fe^{2+} + Mg + Mn- 13.0$

X_{ab}^{pl} is fraction of albite content in plagioclase, X_{an}^{pl} is fraction of anorthite content in plagioclase. Value of Y_{ab} and Y_{ab-an} are automatically calculated and inserted to the function by the software program.

Equation 6 and 8 are based on the edenite-tremolite reaction: 4 quartz + edenite =albite + tremolite. So for applying them existence of quartz is necessary. Equation 7 is based on the edenit-richterite reaction: edenite + albite = richterite + anorthite. Equation 7 for assambelages with or without quartz can be used.

In order to clarify how graphical method works, equations 4-8 are drawn in a P-T diagram (Fig. 3). Data used here are adopted from Sayari [19] related to a microprobe analysis for a pair Amp-Pl coexisting in an andesite sample. One of the advantages of using graphical method is that by plotting equations of interest, it is easy to infer which of the equations are suitable for using to plot. For example in Figure 3 none of equations 6 and 8 are useful to get temperature on the base of plotting with the equation 5 because there is no intersection point in positive range of P. However, applying equation 7 with equation 5 is useful.

According to what is discussed in the graphical method section, the point of intersection of two functions thermometer and barometer reveals the point of crystallization (pressure and temperature) of coexisting Amp-Pl. Functions are plotted in a P-T diagram in which horizontal axis is T (temperature) in degree of centigrade (°C) and vertical axis is P (pressure) in kilobar (kbar). Range of T for drawing can be easily changed by editing in the boxes "From" and "To" (see Fig. 2), so user would be able to read the intersection point in more accuracy by limiting the range of drawing. For example, in Figure 4 the range of temperature of drawing is limited from 0-1000 °C to 800-810 °C.

After entering all required inputs and selecting thermometer and barometer calibrations of interest, the button "Plot" (see Fig. 2 and 4) should be pressed to plot the functions. Thermometer and barometer would be plotted in blue and green color respectively. It must be noticed that after any changes in the inputs, thermometer and barometer calibrations must be reselected before pressing the button "Plot" unless the new changes might not be implemented in the plot.

Values applied as inputs in Figure 2 and 4 are related to a microprobe analysis of a pair Amp-Pl coexisting in the andesite sample of Sayari [19].

APG software program is prepared to run on WINDOWS system operator, and it is also possible to prepare it for LINUX system operator. This software program will be easily achievable through contacting m.sayari@gmail.com and http://www.petrology.ir web site. For calculating formula of amphiboles based on Holland and Blundy [6] and plagioclase to gain required inputs two spread sheet files of Microsoft Excel are accompanied with the APG software. They may be very useful to gain inputs swiftly. Also a word document is accompanied with the APG software which explains how the software should be installed.

Acknowledgements

The author would thank the University of Isfahan for its support and Ph.D. student, Narges Shirdashtzadeh for her review.

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