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APG2: a New Version of APG, an Application for Amphibole-Plagioclase Geothermobarometry

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Abstract

APG2 is a computer application designed for amphibole-plagioclase geothermobarometry. It is the first updated version of APG and supports 4 thermometer models and 6 barometer models involving either amphibole-plagioclase or amphibole only. APG2 has capability to integrate all 4 thermometer models with 6 barometer models and produce 24 different states which user can export them all at once to an Excel table. APG2 works in both graphical and analytical way. APG2 is also able to calculate the H_2O content and Oxygen fugacity (logfO_2) of magma hosting amphiboles.

Keywords: APG2 application; Amphibole; Plagioclase; Geothermobarometry.

Introduction

Estimation of pressure (P) and temperature (T) of petrologic environments has been one of the petrologists' foci [1-9]. Proceeding with this course, petrologists, at first, introduced quality-based methods to the community of petrology. These approaches work on pattern diagrams such as pyroxene thermometry [2]. Next, putting up with advancing experimental petrology and integrating statistical methods, researchers have updated their methods. So the focus of thermobarometry approach was transmuted to quantity-based methods that work numerally, and quantify P and T. They are mathematical equations structured based on statistical regression derived from experimental petrology data. These equations have come to be known as geothermobarometry equations and are divided into two general groups, one-variant and bi-variant equations.

The advantage of bi-variant geothermobarometers is that they work more accurate to estimate P and T, because they do not ignore P or T while trying to estimate other parameter. This advantage is at the cost of getting more complexity. In addition, for calibrating geothermobarometers, a wide variety of relations between content of ions in minerals can be used. The more the equation involves parameters, the more accurate it becomes. Also, in proportion as the equation has more parameters, it becomes more complex. Complexity in the equations may confuse the user, if user does not have a powerful tool to overcome it.

Among the most common geothermobarometry equations, suitable for intermediate magmatic rocks, are amphibole-plagioclase (Amp-Pl) thermometry and amphibole (Amp) thermobarometry. Since amphibole and plagioclase exist 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. Sayari [9] developed an efficient

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software program, named APG, engaging noted thermobarometers related to Amp-Pl. In this paper a more empowered efficient application is introduced for handling Amphibole-plagioclase geothermobarometry equations.

Materials and Methods

Most of the suggested calibrations of geothermobarometers in petrology such as amphibole-plagioclase thermometry [e.g., 10-11], amphibole barometry [e.g., 12-13] clinopyroxene geothermometry and geobarometry [e.g., 14; 6; 15; 7], garnet-clinopyroxene geothermometry [e.g., 1; 16; 17; 18; 19; 20; 8] involve two variants of T and P. These kinds of equations cannot be solved individually. The only way to solve these equations in order to derive P and T is to integrate a pair of them together coincidently. There are two well-known approaches to solve two equations having two shared variants, 1) analytic method 2) graphical method.

In graphical method, it is just enough to draw a couple of geothermobarometry equations of interest in the P-T diagram. These equations are almost bi-variant and P-T dependent. When two equations are plotted in the P-T diagram, the asked P and T are easily obtained from the intersection point of the two equations. When two supposed bi-variant equations are solved together, the result may be unique or not. Even it is possible that no answer appears. This situation clarifies the worth of using graphical method, because graphical method enables user to see which of the situations happens. When more than one intersection point appears in the P-T diagram, choosing the appropriate answer which is in the harmony of petrologic and mineralogical aspects is not very hard.

Results and Discussion

Sayari [9] successfully used graphical method for programing an application, named APG, designed for Amphibole-Plagioclase thermobarometry. APG has been used successfully in petrologic researches [e.g., 21-24]. APG works only in the graphical way.

APG2 is the new version of APG which works not only in the graphical way, but also in the analytical method. In APG2 at the same time that selected geothermobarometry models are drawn, the intersection point of them is calculated analytically and appears on the P-T diagram. If more than one intersection point exists, the only appropriate one is exhibited on the diagram.

Layout of this software program is exhibited in Figure. 1. As it is obvious in Figure. 1, this application

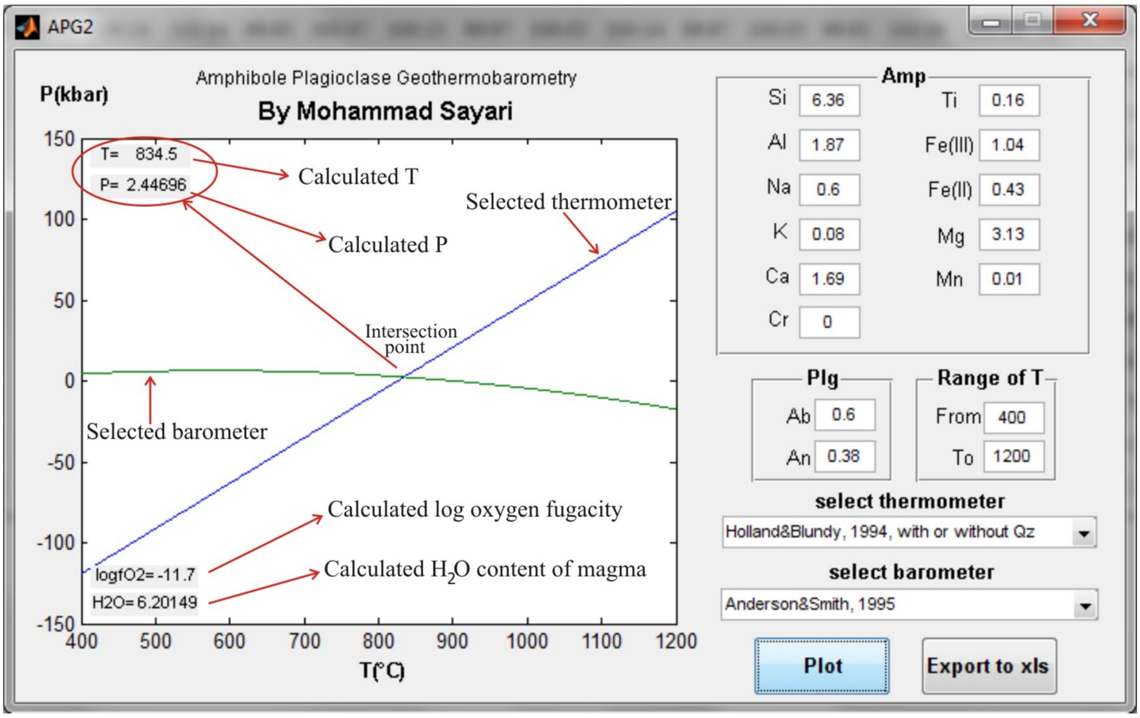

Figure 1. Layout of the APG2 software program. Input data from Sayari [30].

Table 1. An example table of the outputs showing all the results derived from integrating all the models (data are the results of the inputs shown in Figure 1).

Parameter	Equation	Hammarstrom& Zen, 1986	Hollister et al., 1987	Johnson& Rutherford, 1989	Schmidt, 1992	Anderson& Smith, 1995	Ridolfi et al., 2010
P	Holland& Blundy, 1994, with Qz	5.4861	5.7868	4.4501	5.8912	1.758792	2.827149
T	Holland& Blundy, 1994, with Qz	822.3545	819.6838	831.5559	818.7565	855.4591	845.9703
P	Holland& Blundy, 1994, with or without Qz	5.4861	5.7868	4.4501	5.8912	2.446961	2.827149
T	Holland& Blundy, 1994, with or without Qz	845.3395	846.412	841.6444	846.7844	834.4997	835.8557
P	Blundy& Holland, 1990	5.4861	5.7868	4.4501	5.8912	0.096604	2.827149
T	Blundy& Holland, 1990	812.9118	808.0275	829.7398	806.3317	900.4545	856.1017
P	Ridolfi et al., 2010	5.4861	5.7868	4.4501	5.8912	-0.30866	2.827149
T	Ridolfi et al., 2010	910.4936	910.4936	910.4936	910.4936	910.4936	910.4936

has three sections for inputting required data.

1) Amp panel: In this section, composition of Amphibole of interest must be written. All items in this section must be in a.p.f.u. (atom per formula unit). They can be easily gained from structural formula of amphiboles calculated to 23 oxygen atoms [11; 25].

2) Pl panel: In this section, composition of Plagioclase of interest should be entered. This section includes two fields entitled *"Ab"* and *"An"* which implies the Values of albite and anorthite content respectively. These values must be between 0 and 1.

3) Range of temperature (T): This section includes two parameters labeled *"From"* and *"To"* which designate domain of temperature for plotting selected models.

As it is noticeable in Figure. 1 there are two popup menus for selecting barometer and thermometer models. Thermometer popup menu includes 4 most common thermometer models labeled as:

1. *"Holland & Blundy, 1994, with Qz"* implying this model refers to the equation that Holland and Blundy [11] calibrated for situations that existence of quartz is necessary. This model was calibrated based on edenite-tremolite reaction: 4 quartz + edenite =albite + tremolite.

2. *"Holland & Blundy, 1994, with or without Qz"* showing this model referes to the equation that Holland and Blundy [11] calibrated for situations that existence of quartz is not necessary. This model is based on the edenit-richterite reaction: edenite + albite = richterite + anorthite.

3. *"Blundy and Holland, 1990"* indicating that this model refers to the equation represented by Blundy and Holland [10] which was calibrated for edenite-tremolite reaction just like the first model.

4. *"Ridolfi et al., 2010, Amp only"* clarifying this models applies the method of Ridolfi et al. [13] and, unlike 3 other thermometers, engages only amphibole characteristic to estimate T. This model is P-independent and appears in the P-T diagram as a vertical line.

Barometer popup menu includes 6 well-known barometer models labeled as:

1. *"Hammarstrom&Zen, 1986"* showing this model works according to barometer represented by Hammarstrom and Zen [26]. This model is a T-independent function of P.

2. *"Hollister et al., 1987"* referring the use of barometer model of Hollister et al. [27]. This model is also T-independent.

3. *"Johnson&Rutherford, 1989"* implying this model applies barometer model of Johnson and Rutherford [28]. This model is T-independent too.

4. *"Schmidt, 1992"* clarifying method of Schmidt [29] will be applied if this model is selected. This model is also T-independent.

5. *"Anderson&Smith, 1995"* designating that this model performs barometer model of Anderson Smith [12]. Just unlike 4 previous barometer models, this model is T-dependent. It means that it is a bi-variant equation of T and P. Not ignoring the role of T in calibrating this model, This model should be more accurate than the others.

6. *"Ridolfi et al., 2010"* showing this models follows the approach of Ridolfi et al. [13] to estimate P. This model is T-independent and appears in the P-T diagram

as a horizontal line. This barometer works based only on the amphibole analysis. This means using this model does not require plagioclase analysis.

a. Advantages of APG2

Advantages of APG 2, compared to APG, are outlined as bellow:

1. In APG2 two new models are considered. They are thermometers and barometers introduced by Ridolfi et al. [13]. These models are available through pop-up menus of thermometer and barometer in APG2. This characteristic increases the number of combinations from 15 (in APG) up to 24 (in APG2).

2. APG2 runs along both graphical and analytical way, while APG works only in graphical way. In APG2, the coordinate of the intersection point of the thermometer and barometer line/curve which is the answer of the system is calculated through analytical approach and is printed on the P-T diagram.

3. APG2 is enabled to export all the results derived from integrating all the models to a table with xls format readable with Microsoft Excel software. An example of this table is shown as Table 1. In fact, Table 1 is a list of results derived from the inputs shown in Figure 1.

This facility expedites the speed of calculation and comparing results. It means that APG2 has the ability to combine all models, solve them, produce 24 answers and export all the results instantly.

4. The oxygen fugacity and the H_2O content of melt are also calculated based on the way of Ridolfi et al. [13].

b. How to run APG2

APG2 is written in MATLAB and works with Matlab Component Runtime. Before running APG2, user must make sure that MCR 7.8 (Matlab Component Runtime) is installed on the target computer. It is highly important to know that without installing MCR, APG2 will not work. To install MCR, just run MCRInstaller7.8.exe.

After making sure that MCR 7.8 is installed properly on the target computer, user should follow 8 steps below to use APG2 properly.

1. Run APG2.exe to load application.

2. Enter amphibole (Amp) parameters in the Amp panel. All items in this section must be in a.p.f.u. (atom per formula unit). Filling out this panel cannot be skipped.

3. Enter the content of anorthite (An) and albite (Ab) of plagioclase in the Plg panel. Values are required to be in the range of 0-1. If the user is to use the only thermometer *"Ridolfi et al., 2010, Amp only"*, Filling out this panel is not necessary.

4. Enter the range of T (°C) for plotting in the panel labeled *"Range of T"*.

Table 2. Microprobe analyses and structural formula of the pair amphibole-plagioclase phenocrysts in the dacitic rock lying in the Central Iranian Magmatic Arc [30].

Sample	Pair 1		Pair 2		Pair 3		Pair 4		Pair 5	
	Pl	Amp	Pl	Amp	Pl	Amp	Pl	Amp	Pl	Amp
SiO_2	58.95	44.48	58.84	45.51	59.21	45.23	58.8	45.4	58.47	44.01
TiO_2	-	1.46	-	1.82	-	1.8	-	1.87	-	1.48
Al_2O_3	25.53	11.12	25.5	10.41	25.31	10.27	25.43	10.35	25.75	11.31
FeO	0.16	12.32	0.23	10.69	0.2	10.15	0.14	10.69	0.25	12.75
MnO	-	0.11	-	0.05	-	0.07	-	0.12	-	0.1
MgO	-	14.69	-	15.83	-	16.29	-	15.51	-	14.54
CaO	8.08	11.05	8.17	11.13	7.92	11.16	8.16	11.47	8.44	11.14
Na_2O	7.06	2.15	7.03	2.02	7.17	2.17	7.15	2.13	6.72	2.11
K_2O	0.29	0.43	0.3	0.45	0.31	0.46	0.29	0.49	0.3	0.45
BaO	0	0.04	0	0.08	0.03	0.07	0	0.11	0	0.05
Total	100.06	97.85	100.07	97.99	100.15	97.67	99.97	98.15	99.92	97.95
Si	2.64	6.36	2.63	6.45	2.65	6.42	2.63	6.47	2.62	6.3
Al	1.35	1.87	1.34	1.74	1.33	1.72	1.34	1.74	1.36	1.9
Ti		0.16		0.19		0.19		0.2		0.16
Fe^{3+}	0.01	1.04	0.01	0.95	0.01	0.96	0.01	0.72	0.01	1.09
Fe^{2+}	-	0.43	-	0.32	-	0.25	-	0.56	-	0.43
Mn	-	0.01	-	0.01	-	0.01	-	0.01	-	0.01
Mg	-	3.13	-	3.35	-	3.45	-	3.3	-	3.1
Ca	0.39	1.69	0.39	1.69	0.38	1.7	0.39	1.75	0.41	1.71
Na	0.61	0.6	0.61	0.56	0.62	0.6	0.62	0.59	0.58	0.59
K	0.02	0.08	0.02	0.08	0.02	0.08	0.02	0.09	0.02	0.08
Ba	0	0	0	0	0	0	0	0.01	0	0
An (%)	38.11	-	38.45	-	37.24	-	38.07	-	40.27	-
Ab (%)	60.28	-	59.86	-	61.03	-	60.32	-	58	-

5. Select a barometer from the barometer pop-up menu.

6. Select a thermometer from the thermometer pop-up menu.

7. Click on the *"Plot"* button to apply all entered input data and selected methods. Results will be shown on a P-T diagram. Selected thermometer and barometer will be plotted in blue and green respectively. Coordinate of acceptable intersection point will be printed on the top-left side of the P-T diagram. $\log fO_2$ and H_2O content (wt. %) are shown at the bottom-left side of the P-T diagram (Figure. 1).

8. Click on the *"Export"* button to export all the results to a table with xls format. The table will be saved as *"Results.xls"* in the same folder that APG2.exe exists.

While using APG2, it is important to know that after any changes in inputs, user must reselect barometer and thermometer again (steps 5 and 6) then click on *"Plot"* button. Otherwise changes will not be applied. The next important note is that all necessary fields are required to be filled out, even those with zero value; otherwise calculation is going to be wrong. For example, if Mn=0 for Amp, 0 must be typed in the box labeled *"Mn"*.

c. Availability

Both APG2.exe and MCRInstaller7.8.exe are freely available through contacting m.sayari@gmail.com.

d. Practical example

It is already discussed in details how APG2 works. It is just explained how APG2 integrates different models of amphibole-plagioclase thermobarometry and estimates Oxygen fugacity ($\log fO_2$) and the H_2O-content of magma. Now I show how APG2 works with natural samples and illustrate the practical aspects of APG2 through a natural dacitic rock in the central part of the Central Iranian Magmatic Arc known as Urumieh-Dokhtar Magmatic Arc (UDMA). Petrological research shows that this rock is related to the third main Cenozoic volcanic activities specified as the post-collisional adakitic volcanism and is the product of the partial melting of the subducted Arabian slab beneath Eurasian plate [30].

This dacite is mainly composed of euhedral phenocrysts of plagioclase, amphibole, and biotite lying in a groundmass of fine crystals such as feldspar, quartz and opaque, microlite, and glass. The rocks show typical porphyritic textures of volcanic rocks such as hyalo-porphyritic, microlitic-porphyritic, and trachytic textures. Euhedral phenocrysts of amphibole are hornblende type and lie next to tabular plagioclase phenocryst with a normal contact. Since they do not show any evidence of actinolitic margins, the hornblende and plagioclase rims are assumed to represent an equilibrium assemblage. This implies that they are suitable for geothermobarometry investigations to evaluate temperature and pressure of crystalization.

The results of microprobe analyses and structural formula of phenocrysts are presented in Table 2. The calculation of structural formula for amphiboles is done based on 23 oxygen atoms following the 13CNK method [25].

Structural formula of plagioclase were calculated based on 8 oxygen atoms [31]. All analyzed plagioclases are andesine.

The best way to get information from the thermometry and barometry equations is to integrate them [9]. In this case, APG2 was used. All four thermometer equations available in the thermometer popup menu have been integrated with all six barometer equations available in the barometer popup menu. Consequently, 24 different methods for calculating T and P were produced. For illustrating, the results of 2 out of the 24 methods are represented in Table 3.

For the method 1, the 2th thermometer model labeled *"Holland&Blundy, 1994, with or without Qz"* is integrated with the 5th barometer model labeled *"Anderson&Smith, 1995"*. Method 2 integrates thermometer model labeled *"Ridolfi et al., 2010, Amp only"* with the 6th barometer model labeled *"Ridolfi et al., 2010"*. In fact, method 1 uses both amphibole and plagioclase analyses, while method 2 applies only amphibole analyses.

As it is obvious in Table 3, based on the method 1 which involves both plagioclase and amphibole

Table 3. Results of thermobarometry, H_2O-content, and $\log fO2$ derived from APG2 for the dacitic rock lying in the Central Iranian Magmatic Arc [30].

Sample		Pair 1	Pair 2	Pair 3	Pair 4	Pair 5
Method 1	T (°C)	834	833	850	820	855
	P (kbar)	2.45	2	1.4	2.39	1.88
Method 2	T (°C)	910	901	907	905	919
	P (kbar)	2.83	2.35	2.28	2.35	2.95
H_2O (wt.%)		6.20	5.51	5.03	5.39	6.13
$\log fO_2$		-10.2	-11.5	-11	-11.9	-11.3

chemistry, plagioclase and amphibole the phenocrysts crystalized in the temperature range of 820–855 °C and the pressure range of 1.4–2.39 kbar. Method 2, which works only with amphibole chemistry, indicates amphiboles crystalized in the temperature range of 901–919 °C and the pressure range of 2.28–2.95 kbar.

The results of Oxygen fugacity and H_2O-content of magma derived from APG2 for pair samples represented in Table 2 are shown in Table 3. They indicate that H_2O-content of magma was about 5.5 wt% and logfO_2 of magma was about -11.

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