Short note

EASYGRESGRANT—A Microsoft Excel spreadsheet to quantify volume changes and to perform mass-balance modeling in metasomatic systems

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1. Introduction

Gresens’ initial ideas about the mobility/immobility of elements and the gains and losses of material in hydrothermal systems, together with the subsequent isocon method proposed by Grant, have led to the development of a considerable number of mass-balance computer programs for application to metasomatic systems (e.g., Leitch and Day, 1990; Potdevin, 1993; Sturm, 2003; Coelho, 2006). Nevertheless, some of them (NEWGRES or Gresens 92) do not work properly on today’s computers or only work on the Windows platform (SHEARCAL or Geoiso). To date, all mass-balance programs have other problems: (1) graphical plots, such as Grant’s isocon diagram or Gresens’ composition-volume diagram, are not useful tools in order to find immobile elements when a large data set is being handled, since the large number of lines or symbols represented hinders visualization and the distinction of the elements themselves; (2) the method of arbitrary scaling of compositional data proposed to mitigate this problem in the isocon diagram (Grant, 1986) has recently been reported to be inadequate, since scaling influences the best-fit isocon, yielding errors in the mass-balance calculations (Mukherjee and Gupta, 2008).

This short note presents EASYGRESGRANT, a new user-friendly interactive Microsoft Excel spreadsheet program that can be run on the Mac and Windows platforms and that permits correct selection of immobile elements from clusters of slopes, volume factors, and an improved isocon diagram, providing an error-free mass-balance modeling for application in metasomatic systems.

2. Mass-balance applied to hydrothermal systems: a theoretical overview

The absolute mobility of a component \(i\) in a natural system was quantified by Gresens (1967) according to the formula

\[
\Delta m_i = f_v (\rho_a / \rho_0) (C_{i_a} - C_{i_0}),
\]

where \(0\) and \(a\) represent the original and the altered rock, respectively, and \(\rho_0\) and \(\rho_a\) represent densities; \(\Delta m_i\) is the mass change in component \(i\); \(C_{i_0}\) and \(C_{i_a}\) are the initial and final concentrations in component \(i\), respectively, and \(f_v\) is the volume factor or ratio of the final volume to the initial volume. Knowledge of either the geochemical behavior of one element or the \(f_v\) permits the mass balance of this element to be obtained. In practice, there may sometimes be no sound textural or field evidence for assuming a value for \(f_v\) or \(\Delta m_i\). Hence, Gresens (1967) proposed to plot gains and losses as a function of arbitrary volume factors in composition-volume diagrams. By using these diagrams, it is possible to choose a value for \(f_v\) where the curves for several elements (i.e., immobiles) simultaneously cross the gain-loss zero line. This \(f_v\) is the reference frame that is used to estimate the gains and losses of the rest of elements using Eq. (1).

Potdevin (1993) proposed another composition-volume diagram where the gains and losses of elements are plotted with...
respect to their initial contents. Similar to Gresens’ method, the mass balance is carried out by choosing an \( f_v \) from lines that cross the gain-loss zero line.

A simpler graphical method for the solution of Gresens’ equations was proposed by Grant (1986), who rearranged these equations into a linear relationship (the so-called isocon equation) between the concentration of a component in the altered rock and that of the original. The isocon equation is

\[
C_a = \left( \frac{m_0}{m_a} \right) C_0,
\]

(2)

where \( m_0 \) is the reference mass of the original sample, and \( m_a \) is the mass of the altered sample.

In Eq. (2) it is necessary to know the mass change \( \left( \frac{m_0}{m_a} \right) \), which can be calculated graphically by representing the

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**Table 1**

Description of worksheets and main userforms included in EASYGRESGRANT.

<table>
<thead>
<tr>
<th>Name of sheet (S)/userform (U)</th>
<th>Description of the most relevant features</th>
</tr>
</thead>
<tbody>
<tr>
<td>Home (S)</td>
<td>It is the main worksheet. It is automatically activated after starting the program. Navigation in the workbook can be achieved from here and the main modules of the program can be launched. Samples and reference frames to model can be selected.</td>
</tr>
<tr>
<td>Unaltered samples (S)</td>
<td>Spreadsheet where major and trace elements (up to 59) of unaltered samples (up to 52) are input. No numerical data can be deleted automatically.</td>
</tr>
<tr>
<td>Altered samples (S)</td>
<td>Spreadsheet where major and trace elements (up to 59) of altered samples (up to 52) are input. No numerical data can be deleted automatically.</td>
</tr>
<tr>
<td>Isocon graph (S)</td>
<td>In this spreadsheet the ( C_a/C_0 ) diagram shows the isocon, constant volume, or constant mass lines. Major, trace, or a customized selection of elements can be plotted and any element can be temporarily removed from the diagram. Samples and immobile elements to be modeled can be selected/changed. The axis scale of the plot can be modified and the plot can be split into four diagrams at different scales. A regression method is applied to constrain the fit of the isocon.</td>
</tr>
<tr>
<td>Mass-balance numresults (S)</td>
<td>Spreadsheet where mass-balance modeling and changes in mass and volume, where appropriate, obtained from the isocon, clusters of slopes, or volume factors are shown numerically in a table format.</td>
</tr>
<tr>
<td>Mass-balance graphresults (S)</td>
<td>Spreadsheet where mass-balance modeling obtained from the isocon, clusters of slopes, or volume factors are shown graphically in four diagrams. Changes in mass and volume are displayed numerically where appropriate.</td>
</tr>
<tr>
<td>Composition-volume diagrams (S)</td>
<td>In this sheet, Gresens’ and Potdevin’s composition-volume diagrams are plotted to check the selection of immobile elements performed in the cluster of volume factors. Samples, immobile elements, and axis scales can be modified.</td>
</tr>
<tr>
<td>Component-ratio diagram (S)</td>
<td>In this sheet the component-ratio diagram is plotted. The samples and component ratios to be plotted can be selected.</td>
</tr>
<tr>
<td>Cluster of slopes (U)</td>
<td>In this userform, the user selects elements with very close slope values in a cluster of ordered slope values in order to perform the mass-balance modeling. The selection can be checked by means of a least-squares regression method.</td>
</tr>
<tr>
<td>Cluster of volume factors (U)</td>
<td>Userform where the user selects elements with very close volume factor values in a cluster of ordered volume factors in order to carry out the mass-balance modeling. The user can check the selection in composition-volume diagrams.</td>
</tr>
<tr>
<td>Pasted values (S)</td>
<td>Spreadsheet where a compilation of cluster of slopes or volume factors is shown.</td>
</tr>
</tbody>
</table>
concentrations in the altered rock against those in the original and connecting, by means of a straight line through the origin (isocon), the components that show no relative gain or loss of mass (immobile elements). The slope of the isocon line defines the mass change in the alteration, whereas the deviation of a data point from this line represents the concentration change for the corresponding component. The most useful measure of gain or loss is the change in the concentration of a component ($\Delta C_i$) relative to its concentration prior to alteration, leading to the following equation (Grant, 1986):

$$\frac{\Delta C_i}{C_i} = \left( \frac{m_a}{m_0} \right) C_i - 1.$$  

Thus, the mass change of one component is readily obtained by estimating the best-fit isocon, calculating the inverse of the slope and applying Eq. (3).

![Fig. 2](image-url)
When only one element is considered to be immobile, the equation applied to estimate mass change is as follows:

\[ \frac{\Delta C_i}{C_i} = \left( \frac{C_{i0}}{C_i} \right) - 1. \]  
(4)

Similarly, constant mass or constant volume may be assumed to be the reference frame to carry out the mass-balance calculations using, respectively (Grant, 1986).

\[ \Delta C_i = C_i - C_{i0} \]  
(5)

\[ \Delta C_i = \left( \frac{\rho_i}{\rho_{i0}} \right) C_i - C_{i0} \]  
(6)

3. Program structure

The schematic presentation of the EASYGRESGRANT program is given in Fig. 1; a concise description of all worksheets and main userforms is given in Table 1, and the appearance of the worksheets is illustrated in Fig. 2. Further details can be found in the program user manual.

4. Immobile elements as a reference frame for mass-balance modeling

Although some metasomatic processes can sometimes be considered to take place at constant volume or constant mass, often there is no evidence to justify such assumptions, and the immobility of one or some elements must be used as a reference frame for mass-balance modeling. Establishing the immobile element(s) is not always easy. Although several methods have been proposed, all of them can be used in EASYGRESGRANT:

(i) Clusters of slopes and volume factors. This method consists of estimating the slopes and the volume factors for all the elements considered (Grant, 2005; Mukherjee and Gupta, 2008). Clusters of elements with close slope or volume factor values are selected as immobile elements (Fig. 3). The average of these parameters would represent the reference frame for mass-balance computation. Owing to its simplicity and reliability, it is the method suggested for selecting immobile elements. Nevertheless, the computation of the average of these parameters provides no information about the uncertainties due to the selection of elements. To establish them, either statistical approaches or specific plots mentioned above have been used.

(ii) Composition-volume diagrams. These diagrams are not clear when a large data set must be handled. Currently, the excessive number of plotted lines hampers the display of the point where lines representing elements with a similar geochemical behavior intersect (Fig. 4a). In EASYGRESGRANT this problem has been solved by only plotting the immobile elements selected.
previously by means of the clusters of volume factors (Fig. 4b). Thus, here composition-volume diagrams are methods to verify the previous selection of immobile elements.

(iii) The isocron diagram or $C_a/C_0$ diagram. Similar to composition-volume diagrams this diagram can also be used to check the selection of immobile elements previously performed in the uniform clusters of slopes. However, since the $C_a/C_0$ diagram obtained with EASYGRESGRANT plots elements without scaling concentrations and the subsequent stacking of elements is eliminated (e.g., plotting diagrams at different scales, scaling axes, and temporarily removing some elements, Fig. 5a), this diagram can be also used to make the selection of immobile elements. Verification of the selection of immobile elements is carried out by a classical least-squares regression method (Fig. 5b).

(iv) The component-ratio diagram. This diagram plots the ratio of elements of altered and unaltered rocks. Immobile elements appear immediately next to the 1:1 ratio line, whereas mobile elements are plotted away from the line (Fig. 6).

5. Conclusions

EASYGRESGRANT is an Excel worksheet that can be run on the Mac and PC platforms and is based on the Gresens and Grant methods for studying metasomatic systems. The program performs mass-balance calculations considering all possible reference frames: immobile elements, constant volume, and constant mass. The use of clusters of slopes or volume factors to select immobile elements represents an important advantage over classic graphical methods. The averages of the slopes and volume factors offer a reliable reference frame to perform mass-balance calculations. Moreover, the slight modifications made to the $C_a/C_0$ diagram in EASYGRESGRANT would also allow an error-free mass-balance modeling to be made.

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Appendix A. Supporting information

Supplementary data associated with this article can be found in the online version at doi:10.1016/j.cageo.2011.07.014.

References


