The essence of Isocon line and principle for selection of immobile components

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Abstract

Mass balance is of great significance in earth sciences. Isocon method is simple and efficient in mass-transfer calculation. However, problems exist in the identification of immobile components, the choice of the parental sources' compositions, and visualisation. This paper demonstrated that mobility is a relative concept, and the distribution coefficient is the characteristic quantity to describe component mobility. Absolute immobile components are those components with distribution coefficients approaching infinity. The general straight line connecting the origin to the data point of any component carries information on the mass mobility of the component and the evolution degree of the system. Isocon line is a special case of such straight lines. The relationship between final evolved concentrations and the original concentrations is expressed by an equation deduced from mass conservation law and component conservation law, which says the final evolved concentration is determined by the original concentration, distribution coefficient, and the evolution degree. This equation is suitable for all the evolution processes, as long as its mass conserved. Three special Isocon lines were defined, initial Isocon line is the reference line for all the other Isocon lines, absolute Isocon line reflects the evolutionary degree and is formed by absolute immobile components, and relative Isocon line is formed by components having the same/similar distribution coefficients. The components lying on one relative Isocon line are relative immobile to each other, and their ratio equals the original ratio in the initial system. The principle on selection of approximation of absolute immobile components was proposed based on the relationship between the slope and distribution coefficient. A rough knowledge framework on mobility and Isocon analysis was revised and reorganized.

Keywords:

Mass balance, open system evolution, distribution coefficient, Isocon diagram, immobile component

Introduction

Mass balance is of great significance in earth sciences. The evolution of mass is critical to understanding how materials behave in both large-scale and small-scale geologic systems, such as continental collision system and ore-forming system, and how the corresponding compositions and volume evolve over time. Gresens (1967) proposes a general set of equations calculating the gains and losses of components in terms of the chemical analyses and the specific gravities of the unaltered and metasomatized rocks. Two decades later, Grant (1986) modifies his equations into the form solely based on mass, and proposes Isocon method greatly improving the simplicity and efficiency of mass-transfer calculation. And ever since, Isocon diagram becomes a widely used technique to study the material transfers between the evolved products and parental sources. However, there are two main drawbacks in Isocon methods. One is the identification of immobile components (i.e., the identification of Isocon line), especially in the scenario of multiple Isocon lines in progressively evolved progress, the other is the choice of the parental sources' compositions. Additionally, problems exist in the visualisation of Isocon diagram due to the magnitudes of component contents. Because of such drawbacks, a few research papers are published off and on to improve its performance in the last four decades. Baumgartner and Olsen (1995) present a least-square approach to calculate mass transport based on Isocon method. Mukherjee and Gupta (2008) discuss the effect of arbitrary scaling in Isocon method. Guo et al. (2009) introduce a normalization solution to illustrate sequential mass transfers among multiple progressively altered geologic samples. Hilchie et al. (2018) propose a modification of the Isocon diagram to improve the visualization of element behaviour. And Kuwatani et al. (2020) propose a data-driven approach, sparse Isocon analysis, to estimates the mass gains or losses of components without assuming immobile components. All the aforementioned papers focus on how to improve the performance of Isocon diagram, but none fully explains the essence of the Isocon method, such as what Isocon line is and which parameters determine it. As Isocon line is a special straight line passing the origin to data point of immobile component, a more general question is: what is the straight line connecting the origin to the data point of an arbitrary component? Furthermore, the definition of immobile component is relative to the mass, which is an extensive property. The magnitude of the mass is additive and depends on the size of the system, and sometimes it is unable to know the exact value. For example, we are unable to know the exact mass of crust or an ore-forming system of a giant porphyry Cu ore deposit. Consequently, it is necessary to find a scale-independent property to define immobile components. Additionally, the Isocon line is deduced by setting mass transfer ΔC of immobile components as 0, which forms a straight line passing the origin with equation form $C^A = kC^O$. In real applications, however, we follow the opposite logic to choose immobile components, which is to deduce immobile components from the straight lines with equation form $C^A = kC^O$ in the Isocon diagram. These two steps are not equivalent; therefore, it is necessary to find reasonable principles for the selection of immobile components.

The goal of this paper is to find the intrinsic relationship between the final altered concentrations and the original concentrations. First of all, we argued what the immobile components are. Then demonstrated what the general straight line connecting the origin to the data point of an arbitrary component is and what the intrinsic property of Isocon line is. Furthermore, we proposed a general principle for selection of immobile components. And finally, we constructed a rough knowledge framework of mobility. Two applications of forward and inverse models were provided as demos. This paper was organized as follow: section of theoretical deduction demonstrated what immobile component is in mathematics, the relationship between the final evolved/altered consternations and the original consternations, the intrinsic nature of Isocon line, which parameters determinate the Isocon line, and principles for selection of immobile components; section of knowledge framework of mobility provided a rough framework of knowledge on the component mobility and Isocon method discussed in the paper; and section of application cases provided two examples of forward and inverse model demos based on synthetic and real world data sets, respectively.

Theoretical deduction

The assumption is that a homogeneous system consisting of different components initialized with mass of M^O and evolved with two homogeneous subsystems, one is made of materials evolved/altered and remained, and the other made of materials transported away/in (Fig. 1). No mass-energy conversion happened in the whole system. Let's call the former the evolved/altered and remained subsystem, and the latter the transported subsystem. A system is defined as that part of the universe we are interested in. Everything else is defined as surroundings. If the transported subsystem is transported away, then the whole system is a closed system which can exchange energy with surrounding but cannot exchange matter. And if the transported subsystem is transported in, then the whole system is an open system which can exchange both energy and matter with surroundings, i.e., the transported subsystem comes from the surroundings. The components can be in any form, such as element, oxide, mineral, and complex component like N_2O+K_2O. In all evolution processes, the mass of system and each component is conserved. In real-world problem, unfortunately, the evolved/altered and remained subsystem is the only part we can observe undoubtedly, while the initial system and transported subsystem possibly disappeared in geological history, and consequently, we are not able to observe them anymore. For example, during the process of magma differentiation, the crystallized minerals/rocks are the remained subsystem, whereas the evolving melts are the transported-away part. Sometimes we are possibly able to collect unaltered fresh samples of the corresponding rock types in the vicinity of altered rocks of interest to approximate the parental source compositions, but this method is debatable because it is difficult for us to know the real errors between the so-called "fresh samples" and real parental sources. From this point, the evolved/altered and remained subsystem is the primary object in this research. Components are considered as mobile and immobile according to their mass amount in the evolved/altered and remained subsystem and initial system. Mobile components refer to those mass in each subsystem not equal to their mass in the initial system, whereas immobile components refer to those mass in either evolved/altered and remained or transported subsystem equal to their mass in the initial system. However, as mentioned before, mass is an extensive property of system, sometime it is unable to be measured. Therefore, let's first discuss what the immobile component is and try to find a measurable intrinsic property in all situations for it.

What are immobile components?

Let's say the evolved/altered and remained subsystem has mass M^A, and the transported subsystem has mass M^T. The components of interests have bulk concentrations of C^O in the initial system, C^A in the evolved/altered and remained subsystem, and C^T in the transported subsystem, respectively

(Fig. 1). All the variables of a specific component *i* would be denoted by subscript, like M_i^O and C_i^O.

According to the mass conservation law and component conservation law, we have:

$$M^O = M^A + M^T \quad where\ M^O > 0, M^A > 0, and\ M^T > -M^A \quad (1)$$

$$C_i^O M^O = C_i^A M^A + C_i^T M^T \quad where\ C_i^O > 0, C_i^A \geq 0, and\ C_i^T \geq 0 \quad (2)$$

If $M^T > 0$, the initial system involves into two separate subsystems and the mass depletes in the altered and remained system, if $M^T = 0$, the mass of the initial system and the evolved/altered and remained subsystem keeps unchanged, and if $0 > M^T > -M^A$, the initial system involves with the subsystem transported together into the evolved/altered and remained subsystem and the total mass of the system gains. The minus and plus signs of M^T represent the mass transportation direction of the transported subsystem, - for transported-in and + for -away, respectively. In general, M^O and M^T are unknown as they possibly existed only in the past or the depth of Earth and we cannot observe them in real world.

Rearrange equation (2) to:

$$C_i^A = C_i^O \frac{M^O}{M^A} - C_i^T \frac{M^T}{M^A} \quad where\ C_i^O > 0, C_i^A \geq 0, and\ C_i^T \geq 0 \quad (3)$$

C_i^A means the concentration of component *i* in the evolved/ altered and remained subsystem, which is possibly the only variable we can observe in most situations. As the real mass of geologic subsystem exceeding certain large volume is difficult for us to know.

Define the **system mass increment** ΔM as:

$$\Delta M = M^A - M^O \quad where\ \Delta M \in R \quad (4)$$

If $\Delta M > 0$, the mass of the whole system is gained, if $\Delta M = 0$, the mass of the whole system is unchanged, and if $-M^O < \Delta M < 0$, the mass of the whole system is depleted. From equation (1), we know $\Delta M = -M^T$.

Assuming component *i* is immobile, which has two possible situations. One is the total mass of component *i* conserved in the evolved/altered and remained subsystem, and the other is its total mass conserved in the transported subsystem. For the former situation, the mass of component *i* in the evolved/altered and remained subsystem ought to stay exactly the same as its mass in the initial system, and so does the mass of component *i* in the transported subsystem for the latter situation in mathematics. In the perspective of geology, its mass in the evolved/altered and remained or transported subsystem ought to be almost the same as it in the initial system, that means that M_i^A or M_i^T ought to extremely closely approach M_i^O. Define **mass increment of component *i*** ΔM_i as the difference between the mass of component *i* in the evolved/altered and remained subsystem and initial system. Therefore, for the former situation, we have:

$$\Delta M_i = \lim_{M_i^A \to M_i^O} (M_i^A - M_i^O) = 0 \quad (5)$$

According to equation (1):

$$M_i^T = \lim_{M_i^A \to M_i^O} (M_i^O - M_i^A) = 0 \quad (6)$$

Then the concentration of component *i* in the transported subsystem would be:

$$C_i^T = \lim_{M_i^T \to 0} \frac{M_i^T}{M^T} = 0 \quad (7)$$

And for the latter situation,

$$\Delta M_i = \lim_{M_i^T \to M_i^O} [(M_i^O - M_i^T) - M_i^O] = -M_i^O \quad (8)$$

$$M_i^T = \lim_{M_i^A \to M_i^O} [M_i^O - (M_i^O - M_i^T)] = M_i^O \quad (9)$$

Then the concentration of component *i* in the evolved/altered and remained subsystem would be:

$$C_i^A = \lim_{M_i^A \to 0} \frac{M_i^A}{M^A} = 0 \quad (10)$$

Equation (7) says if component *i* is immobile in the evolved/altered subsystem, its concentration in the transported subsystem will equal 0 in mathematics, which means any component detected in the transported subsystem is not immobile in the evolved/altered and remained subsystem. And in real geologic observation, its concentration in the transported subsystem ought to closely approach 0 if its mass is conserved in the evolved/altered and remained subsystem. Equation (10) says if component *i* is immobile in the transported subsystem, its concentration in the evolved/altered and remained subsystem ought to equal 0 in mathematics, which means any component detected in the evolved/altered subsystem is not immobile in the transported subsystem. And in real geologic observation, its concentration in the evolved/altered and remained subsystem ought to closely approach 0 if its mass is conserved in the transported subsystem.

Define **distribution coefficient D** as the ratio of concentrations in the corresponding subsystems. Thus, if the mass of component *i* is conserved in the evolved/altered and remained subsystem, then

$$D_i^{A-T} = \frac{C_i^A}{C_i^T} = \lim_{C_i^T \to 0^+} \frac{C_i^A}{C_i^T} = +\infty \quad (11)$$

and,

$$D_i^{T-A} = \frac{1}{D_i^{A-T}} = \frac{C_i^T}{C_i^A} = \lim_{C_i^T \to 0^+} \frac{C_i^T}{C_i^A} = 0 \quad (12)$$

If the mass of component *i* is conserved in the transported subsystem,

$$D_i^{A-T} = \frac{C_i^A}{C_i^T} = \lim_{C_i^A \to 0^+} \frac{C_i^A}{C_i^T} = 0 \quad (13)$$

and,

$$D_i^{T-A} = \frac{1}{D_i^{A-T}} = \frac{C_i^T}{C_i^A} = \lim_{C_i^A \to 0^+} \frac{C_i^T}{C_i^A} = +\infty \quad (14)$$

As both C_i^A and $C_i^T \geq 0$, when C_i^T approaches 0, D_i^{A-T} would approach positive infinity $+\infty$ and D_i^{T-A} would equal 0, and when C_i^A approaches 0, D_i^{A-T} would approach 0 and D_i^{T-A} would equal positive infinity $+\infty$, theoretically. Equation (11) and (13) say that the distribution coefficients of immobile components are positive infinity $+\infty$ (in the ratio of concentration in the evolved/altered and remained subsystem to concentration in the transported subsystem) or 0 (in the ratio of concentration in the transported subsystem to concentration in the evolved/altered and remained subsystem) in mathematics. Theoretically, only the components observed with distribution coefficient equal to positive infinity $+\infty$ or 0 can be determined as immobile in a geologic evolution system. **D_i^{A-T} approaching positive infinity $+\infty$ (i.e., the mass of component *i* conserved in the evolved/altered and remained subsystem, where $D_i^{T-A} = 0$) means any component with a limited distribution coefficient value is not immobile in the evolved/altered and remained subsystem, and D_i^{A-T} equal to 0 (i.e., the mass of component *i***

is conserved in the transported subsystem, where $D_i^{T-A} = +\infty$) means any component observed in evolved/altered and remained subsystem is not immobile in the transported subsystem. If we stick to mathematics strictly, it may be very difficult to find immobile components. Hence, to solve real-world problems, let's flexibly define components with D_i^{A-T} extremely large or extremely close to 0 as approximations of immobile components. Therefore, from the perspective of geology, **the immobile components can be defined as components with extremely large or small distribution coefficient in a specific geologic evolution system**. Distribution coefficients is a better property to describe mobility than mass, as it is scale-independent and readily measured, either experimentally or observationally. Problems also occur in the definition of "extremely large" and "extremely small", as we don't know how "extremely large" the distribution coefficient is can be described as close enough to infinity, and how "extremely small" can be described as close enough to 0. Anyway, a general criterion for immobile component is either distribution coefficient >> 1 or 0 < distribution coefficient << 1. Such feature is similar to conventional compatible and incompatible components. Components with extremely large distribution coefficients are subsets of compatible component set, while components with extremely small distribution coefficient are subsets of incompatible component set. This explains the reason that REE, Zr, Al_2O_3, and other components are often observed immobile in many researches. Equations (11) and (13) also indicate that **"immobility" is a relative concept. Components immobile in the evolved/altered and remained subsystem are absolute mobile in the transported subsystem, and vice versa**. The terms "mobile" and "immobile" have meaning only when the system is specified.

The essence of Isocon line

Grant (1986) proposed Isocon method by revising Gresens' Equation (1967). However, the Isocon equation can also be derived according to the component conservation law. The derivation process is as follow:

The mass increment of component *i* would be:

$$\Delta M_i = C_i^A M^A - C_i^O M^O \quad where\ \Delta M_i \in R, \Delta M_i \geq -M_i^O \quad (15)$$

To describe mass change rate of the whole system, let's define **system evolution degree** as the ratio of the mass of the evolved/altered and remained subsystem to the mass of initial system.

$$\varepsilon = \frac{M^A}{M^O} \quad where\ M^O > 0, M^A \geq 0, \varepsilon \geq 0 \quad (16)$$

Where Greek letter ε denotes for E in the "evolution". The range of ε is $[0, +\infty)$. If $\varepsilon > 1$, the evolved/altered and remained system mass is gained relative to the initial system, if $\varepsilon = 1$, the evolved/altered and remained system mass is unchanged relative to the initial system, and if $1 > \varepsilon \geq 0$, the evolved/altered and remained system mass is depleted relative to the initial system.

Divide both sides of equation (15) by M^O,

$$\Delta C_i = \frac{\Delta M_i}{M^O} = C_i^A \frac{M^A}{M^O} - C_i^O \quad where\ \Delta M_i \geq -M_i^O, M^O > 0, \Delta C_i \geq -C_i^O \quad (17)$$

The range of ΔC_i is $[-C_i^O, +\infty)$. If $\Delta C_i > 0$, the mass of component *i* in the evolved/altered and remained system is gained relative to the initial system, if $\Delta C_i = 0$, the mass of component *i* in the evolved/altered and remained system is unchanged relative to the initial system, and if $-C_i^O \leq \Delta C_i < 0$, the mass of component *i* in the evolved/altered and remained system is depleted relative to the initial system. Although ΔC_i is critical in the derivation of Isocon line, its meaning is not elucidated in Grant's (1986) paper. Although he simply states it as "the change in concentration of species 'i'" in a later paper (Grant, 2005), the interpretation is inaccurate. As the change in concentration of specie i should be $C_i^A - C_i^O$, rather than $C_i^A \frac{M^A}{M^O} - C_i^O$. Let's return to the original equation $\Delta C_i = \frac{\Delta M_i}{M^O}$, which says ΔC_i is a dimensionless/characteristic quantity derived by dividing the total mass of the initial system M^O into the mass increment of component i. Therefore, it means the mass increment of component i per unit mass of the initial system. From this perspective, let's **define ΔC_i as unit mass increment of component *i* to describe the mass increment of specific component *i* relative to the unit mass of initial system**.

Substitute $\frac{M^A}{M^O}$ in the equation (17) with the left hand of equation (15), then

$$\Delta C_i = \varepsilon C_i^A - C_i^O \quad where\ C_i^A \geq 0, C_i^O > 0, \varepsilon \geq 0, \Delta C_i \geq -C_i^O \quad (18)$$

For arbitrary component i, its concentration in the evolved/altered and remained subsystem is:

$$C_i^A = \frac{M_i^A}{M^A} = \frac{M_i^O + \Delta M_i}{M^A} = \frac{C_i^O + \Delta C_i}{\frac{M^A}{M^O}} = \frac{M^O}{M^A}\left(C_i^O + \Delta C_i\right) = \frac{1}{\varepsilon}\left(C_i^O + \Delta C_i\right) \quad where\ C_i^A \geq 0, C_i^O > 0, \varepsilon \geq 0, \Delta C_i \geq -C_i^O \quad (19)$$

Equation (19) is Grant's equation of C_i^A. Assuming component i is immobile, then equation (19) becomes:

$$C_i^A = \frac{M^O}{M^A} C_i^O = \frac{1}{\varepsilon} C_i^O \quad where\ \varepsilon \geq 0 \quad (20)$$

Equation (20) is Grant's equation of Isocon line, it fits the slope – intercept form of a straight line. Based on it, he thinks any observed concentrations of two or more immobile components would form a straight line in the plot of observed concentrations against their corresponding original/reference concentrations (i.e., Isocon diagram, Fig. 2-a). The straight line expressed by equation (20) is called Isocon, and the components fall on the straight line is determined as immobile components. The logic so far is right; however, the logic is quite the opposite in the application of Isocon analysis. We firstly fit straight lines in the Isocon diagram originating from the origin, and then determine such straight lines as Isocon lines, and components falling on the lines are candidate immobile components. **Here comes the logic problem, as that component *i* is immobile is sufficient condition for equation (20), but not necessary.** In other word, equation (20) does not imply that "component i is immobile" is true. The proof is as follow:

P: component *i* is immobile.

Q: C_i^A is in linear relationship with C_i^O, and the intercepts are 0.

If P is true, then Q is true. This is already demonstrated by the derivation of Equation (19) to Equation (20). Therefore, **P is sufficient for Q**.

The logic problem in the application of Isocon analysis can be questioned as: if Q is true, is P true?

Assuming component i is mobile and its mass increment ΔM_i equals λ_i times its original mass M_i^O, then

$$\Delta M_i = \lambda_i M_i^O \quad where\ \Delta M_i \geq -M_i^O \quad (21)$$

Divide both sides of equation (21) by M^O, easy to know:

$$\Delta C_i = \lambda_i C_i^O \quad where\ \Delta C_j \geq -C_j^O \quad (22)$$

Substitute ΔC_i in the equation (19) with the right hand of equation (22), then

$$C_i^A = \frac{1+\lambda_i}{\varepsilon} C_i^O \ where\ \lambda_j \geq -1, \varepsilon \geq 0 \quad (23)$$

Although component *i* is mobile in this scenario, equation (23) also fits the slope - intercept form of straight lines with 0 intercepts like equation (20). Therefore, **P is not necessary for Q**. Consequently, not all straight lines originating from the origin in Isocon diagram are formed by immobile components. Grant (1986) also noticed a type of such phenomenon in progressively altered samples, Guo et al. (2019) proposed a normalization solution to deal with it. However, this problem is not only happened in progressively altered processes, but also happened in a more general situation when two or more components have the same/similar λ , even in single evolution/alteration stage. As equation (23) is the general form of straight lines originating from the origin and passing the data points in the Isocon diagram, it says **many "Isocon" lines can be formed as long as the coefficients λ of any two or more components are the same/similar, and λ = 0 (i.e., $\Delta C_i = 0, \Delta M_i = 0$) is just one member of the solution set.** When solving real-world problem, it is difficult for us to know the real λ of each component and tell the difference between "mobile" and "immobile" components from a simple Isocon diagram, and we have to regard all the straight lines originating from the origin as possible Isocon lines.

As λ is important in equation (23), let's define λ_i as **relative mass change rate of component *i***, then

$$\lambda_i = \frac{\Delta M_i}{M_i^O} = \frac{\Delta C_i}{C_i^O} \quad where\ \lambda_j \geq -1\ (24)$$

Equation (24) says λ_i is the mass increment per unit mass of component *i* in the initial system, its range is $[-1, +\infty)$, and $\lambda_i = -1$ represents all the mass of specific component *i* were transported away from the initial system, and no longer exist in the evolved/altered and remained subsystem. λ_i describes how much mass changed per unit mass of component *i* in the initial system**.**

Factors determining the Isocon line

As λ_i is difficult to know, let's dig deeper to see what factors determining the Isocon line. Substitute ΔC_i in the equation (24) with the right hand of equation (18), then the relative mass change rate λ_i of component *i* becomes:

$$\lambda_i = \varepsilon \frac{C_i^A}{C_i^O} - 1 \quad where\ \varepsilon\ and\ \lambda_j \geq -1 \quad (25)$$

Define altered and remained factor of component *i* as K_i^A,

$$K_i^A = \frac{C_i^A}{C_i^O} \quad where\ K_i^A \geq 0 \quad (26)$$

Substitute $\frac{C_i^A}{C_i^O}$ in the equation (25) with K_i^A, then

$$\lambda_i = \varepsilon K_i^A - 1 \quad (27)$$

Define transported factor of component *i* as K_i^T,

$$K_i^T = \frac{C_i^T}{C_i^O} \quad where\ K_i^T \geq 0 \quad (28)$$

then,

$$K_i^T = \frac{1 - K_i^A \varepsilon}{1 - \varepsilon} \quad where\ K_i^T \geq 0 \quad (29)$$

Divide equation (26) by equation (28),

$$\frac{K_i^A}{K_i^T}=\frac{C_i^A}{C_i^T} \quad where\ \frac{K_i^A}{K_i^T}\geq 0 \quad (30)$$

The right hand of equation (30) is the definition of distribution coefficient D_i^{A-T}. Therefore,

$$D_i^{A-T}=\frac{K_i^A}{K_i^T} \quad where\ D_i^{A-T}\geq 0 \quad (31)$$

$$D_i^{T-A}=\frac{1}{D_i^{A-T}}=\frac{K_i^T}{K_i^A} \quad where\ D_i^{T-A}\geq 0 \quad (32)$$

Substitute K^T in the equations (31) and (32) with the right hand of equation (29),

$$D_i^{A-T}=\frac{K_i^A(1-\varepsilon)}{1-K_i^A\varepsilon} \quad where\ \varepsilon\neq\frac{1}{K_i^A}\ and\ \varepsilon\geq 0\ (33)$$

$$D_i^{T-A}=\frac{1-K_i^A\varepsilon}{K_i^A(1-\varepsilon)} \quad where\ \varepsilon\neq 1\ and\ \varepsilon\geq 0\ (34)$$

Move K_i^A in equations (33) and (34) to the left hand,

$$K_i^A=\frac{D_i^{A-T}}{(D_i^{A-T}-1)\varepsilon+1} \quad where\ D_i^{A-T}\neq 1-\frac{1}{\varepsilon}\ and\ \varepsilon\geq 0 \quad (35)$$

$$K_i^A=\frac{1}{(1-D_i^{T-A})\varepsilon+D_i^{T-A}}\ (36)$$

Replace K_i^A in equation (27) with the left hand of equation (35):

$$\lambda_i=\varepsilon\frac{D_i^{A-T}}{(D_i^{A-T}-1)\varepsilon+1}-1 \quad where\ D_i^{A-T}\geq 0,\varepsilon\geq 0 \quad (37)$$

Replace K_i^A in equation (27) with the left hand of equation (36):

$$\lambda_i=\varepsilon\frac{1}{(1-D_i^{T-A})\varepsilon+D_i^{T-A}}-1 \quad where\ D_i^{T-A}\geq 0,\varepsilon\geq 0 \quad (38)$$

Replace λ_i in equation (23) with the left hand of equation (37):

$$C_i^A=\frac{D_i^{A-T}}{(D_i^{A-T}-1)\varepsilon+1}C_i^O \quad where\ D_i^{A-T}\geq 0,\varepsilon\geq 0\ (39)$$

Replace λ_i in equation (23) with the left hand of equation (38):

$$C_i^A=\frac{1}{(1-D_i^{T-A})\varepsilon+D_i^{T-A}}\ C_i^O\ where\ D_i^{T-A}\geq 0,\varepsilon\geq 0\ (40)$$

Equations (39) and (40) describe the relationship between the final evolved/altered concentration of component *i* and its original concentration, which say that **the final evolved/altered concentration is determined by the original concentration C_i^O, distribution coefficient D, and the evolution degree *ε*.** The equations fit the slope - intercept forms of straight lines, and the slope is in **nonlinear relationship** with **distribution coefficient D** and the **evolution degree *ε*. Connecting the data point of any component to the origin forms a straight line whose slope carries information about the mass mobility of the component and the evolution degree of the system**. **For a certain evolution degree *ε*, all the components with the same/similar distribution coefficient D would form one straight line passing the origin and data points (Fig. 2-b).** To differ the Isocon lines formed by immobile components from the straight lines formed by mobile components with the same/similar distribution D, let's **define the straight line formed by components with distribution coefficient D equal to/close to ∞ as absolute Isocon line(or Isocon line)**. With such definition, **the slope of Isocon line solely reflects the evolutionary degree**, and **samples with different evolution/alteration degree**

would form different Isocon lines (Fig. 2-b). Grant (1986) explains the meaning of Isocon line as "a line connecting points of equal geochemical concentration" (Gary et al., 1974, p. 374), which is not true/accurate if we check the concentrations of components lying on the Isocon line, whereas the genuine meaning is "**a line connecting points of conserved/unchanged mass**".

If D_i^{A-T} approaches $+\infty$ (i.e., D_i^{T-A} approaches 0), then equations (39) and 40 become:

$$C_i^A = \lim_{D_i^{A-T}\to+\infty} \frac{D_i^{A-T}}{(D_i^{A-T}-1)\varepsilon+1} C_i^O = \lim_{D_i^{A-T}\to+\infty} \frac{1}{(D_i^{A-T}-1)\varepsilon/D_i^{A-T}+1/D_i^{A-T}} C_i^O = \frac{1}{\varepsilon} C_i^O \quad (41)$$

$$C_i^A = \lim_{D_i^{T-A}\to 0} \frac{1}{(1-D_i^{T-A})\varepsilon+D_i^{T-A}} C_i^O = \frac{1}{\varepsilon} C_i^O \quad (42)$$

If D_i^{A-T} approaches 0 (i.e., D_i^{T-A} approaches $+\infty$), then equations (39) and 40 become:

$$C_i^A = \lim_{D_i^{A-T}\to 0} \frac{D_i^{A-T}}{(D_i^{A-T}-1)\varepsilon+1} C_i^O = 0C_i^O \quad (43)$$

$$C_i^A = \lim_{D_i^{T-A}\to+\infty} \frac{1}{(1-D_i^{T-A})\varepsilon+D_i^{T-A}} C_i^O = 0C_i^O \quad (44)$$

Equations (41) and (42) say that **if immobile component *i* is conserved in the evolved/altered and remained subsystem, the plot of C_i^A against C_i^O would form a straight line obliquely intersecting the abscissa with zero intercept, and its slope reflects the system evolutionary degree. If samples experienced different evolutionary degrees, they would form multiple different Isocon lines (Fig. 2-a). All the Isocon lines are meaningful as they reflect to what extent the samples forming the Isocon lines are evolved.** To emphasize such property, we need define a special Isocon line indicating the samples with no change. That would be the Isocon line formed by plotting original concentrations against original concentrations, which is a straight line with slope equal to 1 and 0 intercepts.

$$C_i^A = C_i^O \quad (45)$$

Let's call the Isocon line $C_i^A = C_i^O$ **initial Isocon line**, as **it reflects the mass of all components and the whole system is unchanged** (Fig 2-a)**.** All the components fall on the initial Isocon line, and therefore, the initial Isocon line stands for the initial state of the mass of each component and the whole system. Isocon lines under the initial Isocon line indicate system mass gain (i.e., $\frac{1}{\varepsilon} < 1$), whereas Isocon lines above the initial Isocon line indicate system mass loss (i.e., $\frac{1}{\varepsilon} > 1$).

Equations (43) and (44) say that if immobile component *i* is conserved in the transported subsystem, the plot of C_i^A against C_i^O would **form a straight line parallel to the abscissa (Fig. 2-c)**. As mentioned before, component immobile in the transported subsystem is actually mobile in the evolved/altered and remained subsystem. For those straight line formed by mobile components with non-infinity distribution coefficient D, let's call them "**relative Isocon line**", as **those components lying on them are relative immobile to each other in the evolution processes**, and we can call those components "**relative immobile component pair**" (Fig. 2-b). This is readily demonstrated by supposing that both mobile components *i* and *j* in the same sample have the same/similar distribution coefficients. The concentrations of component *i* and *j* would be:

$$C_i^A = \frac{D_i^{A-T}}{(D_i^{A-T}-1)\varepsilon+1} C_i^O \quad (46)$$

$$C_j^A = \frac{D_i^{A-T}}{(D_i^{A-T}-1)\varepsilon+1} C_i^O \quad (47)$$

As they are in the same sample, hence the evolution degree ε is the same, and their ratio is:

$$\frac{C_j^A}{C_i^A} = \frac{C_j^O}{C_i^O}\frac{D_j^{A-T}}{D_i^{A-T}}\frac{D_i^{A-T}\varepsilon + 1 - \varepsilon}{D_j^{A-T}\varepsilon + 1 - \varepsilon} \xrightarrow{D_i^{A-T} \cong D_i^{A-T}} \frac{C_j^A}{C_i^A} \cong \frac{C_j^O}{C_i^O} \quad (48)$$

Equation (48) says **the ratio of two arbitrary component's evolved/altered concentrations is determined by their original concentrations, distribution coefficient, and evolutionary degree**. Because relative immobile component pair has the same/similar distribution coefficients, **their evolved/altered concentration ratio equals their original concentration ratio**. In other word, **as long as any two components have the same/similar distribution coefficient, they would form one relative Isocon line** (Fig. 2-b)**.** Therefore, many relative Isocon lines can be found possibly in a real-word problem. Due to such feature, relative immobile component pair can be used as trace and discrimination tools of prenatal sources/geologic processes.

Substitute λ_i in the equation (21) with the right hand of equation (37),

$$\Delta M_i = \frac{1-\varepsilon}{(1 - D_i^{A-T})\varepsilon - 1} M_i^O \quad (49)$$

Divide both sides of equation (49) by M^O,

$$\Delta C_i = \frac{1-\varepsilon}{(1 - D_i^{A-T})\varepsilon - 1} C_i^O \quad (50)$$

Substitute D_i^{A-T} in the r equation (49) and (50) with the $D_i^{A-T} = \frac{1}{D_i^{T-A}}$,

$$\Delta M_i = \frac{(\varepsilon - 1)D_i^{T-A}}{(1 - D_i^{T-A})\varepsilon + D_i^{T-A}} M_i^O \quad (51)$$

$$\Delta C_i = \frac{(\varepsilon - 1)D_i^{T-A}}{(1 - D_i^{T-A})\varepsilon + D_i^{T-A}} C_i^O \quad (52)$$

Equations (49) and (51) say the mass increment of component *i* is determined by **its initial mass $\boldsymbol{M_i^O}$, distribution coefficient D**, and the **evolution degree $\boldsymbol{\varepsilon}$**. And correspondingly, equations (49) and (51) say the unit mass increment of component *i* is determined by **its initial concentration $\boldsymbol{C_i^O}$, distribution coefficient D**, and the **evolution degree $\boldsymbol{\varepsilon}$**.

Principle for selection of immobile components

The selection of immobile components is critical in Isocon analysis. Several methods for determination of immobile components are summarized as: i) the clustering of the slope $\frac{C_i^A}{C_i^O}$; ii) a best-fit linear array through the origin on the Isocon diagram, which is the graphical equivalent of the first method, iii) priori assumption of certain immobile components, iv) the assumption of constant mass during evolution, or v) the assumption of constant volume during evolution (Grant, 2005). The first two methods are actually equivalents of the original method choosing immobile components, i.e., inspection on the Isocon diagram, which involves the best fit of a straight line through a series of data points (Grant, 1986). However, the best-fit straight line does not guarantee that the components forming the straight line are immobile. Because the performance of linear regression depends on the distribution of $\frac{C_i^A}{C_i^O}$ data, rather than component's mobility. As we demonstrated before, the slope $\frac{C_i^A}{C_i^O}$ is determined by the distribution coefficient and evolutionary degree in a nonlinear way. Given certain evolutionary degree, the slope $\frac{C_i^A}{C_i^O}$ is solely determined by distribution coefficient. Therefore, the performance of linear regression (i.e., methods i and ii) depends on the distribution of distribution coefficients of components of interest. If the deviation of different component's distribution coefficients is smaller, the linear regression will get a better fit. Other methods are based on assumptions, which are also debatable. Additionally, for a better determination of possible immobile components, some techniques are proposed to improve the visualization of Isocon diagram (Guo et al., 2009; Hilchie et al., 2018).

As proved previously, the essential property determining the mobility of components is the distribution coefficient D. Therefore, the only criterion for selecting immobile components is the distribution coefficient D. As the evolved/altered and remained subsystem is the only part we can observe, thus we want find the absolute immobile components conserved in this subsystem, or some nearly immobile components as approximations. Recall immobile components in the evolved/altered and remained subsystem have distribution coefficient approaching positive infinity, and consequently, **the larger the distribution coefficients (D^{A-T}) of the candidate components we select, the better the approximation is**. If the distribution coefficients of the transported subsystem relative to the evolved/altered and remained subsystem (i.e., D^{T-A}) are available, then **the smaller the distribution coefficients are, the better the approximation is**.

The distribution coefficient is the only property deserving consideration in the choice of immobile components. Hence, let's see how the slope behaves with the distribution coefficient change. According to the equation (39), we know the slope is,

$$k = \frac{C_i^A}{C_i^O} = \frac{D_i^{A-T}}{(D_i^{A-T} - 1)\varepsilon + 1}, where\ k \geq 0 \quad (53)$$

Equation (53) says that the slope k is in a complex nonlinear relationship with distribution coefficient D_i^{A-T} and evolutionary degree ε (Fig. 3-a). Its partial derivative relative to D_i^{A-T} is,

$$\frac{\partial k}{\partial D^{A-T}} = \frac{1-\varepsilon}{(\varepsilon D^{A-T} - \varepsilon + 1)^2}, \qquad where\ D^{A-T} \neq 1 \quad (54)$$

If $\varepsilon < 1$, then $\frac{\partial k}{\partial D^{A-T}} > 0$, and k increases as D^{A-T} increases (Fig. 3-b). If $\varepsilon > 1$, then $\frac{\partial k}{\partial D^{A-T}} < 0$, and k decreases as D^{A-T} increases (Fig. 3-c). If $\varepsilon = 1$, then $\frac{\partial k}{\partial D^{A-T}} = 0$, and k does not change as D changes (Fig. 3-d).

Now let's see how evolutionary degree ε behaves with the distribution coefficient change. Move ε in the equation (39) to the left hand, we have,

$$\varepsilon = \frac{C_i^O D^{A-T} - C_i^A}{C_i^A (D^{A-T} - 1)} \quad where\ D^{A-T} \neq 1, C_i^A \geq 0, C_i^O > 0 \quad (55)$$

Equation (53) says that the evolutionary degree ε is also in a complex nonlinear relationship with distribution coefficient D_i^{A-T}, original concentration C_i^O and evolved/altered concentration C_i^A (Fig. 4). Its partial derivative relative to D_i^{A-T} is,

$$\frac{\partial \varepsilon}{\partial D^{A-T}} = \frac{C_i^A - C_i^O}{C_i^A (D^{A-T} - 1)^2}, \ where\ D^{A-T} \neq 1, C_i^A \geq 0, C_i^O > 0 \quad (56)$$

No matter what value $D^{A-T} (Condition: D^{A-T} \neq 1)$ is, the behavior of ε depends only on the relationship between the evolved/altered concentration C_i^A and original concentration C_i^O. If $C_i^A = 0$, we will not detect component i in the evolved/altered and remained subsystem, so it is not necessary to consider such situation in reality. If $C_i^A > C_i^O$ ($i.e.,$ $\varepsilon < 1$), then $\frac{\partial\varepsilon}{\partial D^{A-T}} > 0$, and thus ε increases as D^{A-T} increases (Fig. 4 -a and -b). If $C_i^A < C_i^O$ ($i.e.,$ $\varepsilon > 1$), then $\frac{\partial\varepsilon}{\partial D^{A-T}} < 0$, and thus ε decreases as D^{A-T} increases (Fig. 4 -c and -d). If $C_i^A = C_i^O$($i.e.,$ $\varepsilon = 1$), then $\frac{\partial\varepsilon}{\partial D^{A-T}} = 0$, ε does not change with D^{A-T}.

The second-order partial derivative of ε relative to D^{A-T} is,

$$\frac{\partial^2\varepsilon}{\partial^2 D^{A-T}} = \frac{2(C_i^O - C_i^A)}{C_i^A(D^{A-T}-1)^3}, \qquad where\ D^{A-T} \neq 1, C_i^A \geq 0, C_i^O > 0 \quad (57)$$

If $D^{A-T} > 1$, then $(D^{A-T}-1)^3 > 0$. When C_i^A is larger than C_i^O ($i.e., C_i^A > C_i^O$, $\varepsilon < 1$), $\frac{\partial^2\varepsilon}{\partial^2 D^{A-T}}$ would be smaller than 0 ($\frac{\partial^2\varepsilon}{\partial^2 D^{A-T}} < 0$), the graph of ε is concave downward relative to D^{A-T} (Fig. 4-a); when C_i^A is smaller than C_i^O ($i.e., C_i^A < C_i^O$, $\varepsilon > 1$), $\frac{\partial^2\varepsilon}{\partial^2 D^{A-T}}$ would be larger than 0 ($\frac{\partial^2\varepsilon}{\partial^2 D^{A-T}} > 0$), the graph of ε is concave upward (Fig. 4-c).

If $D^{A-T} < 1$, then $(D^{A-T}-1)^3 < 0$. When C_i^A is larger than C_i^O ($i.e., C_i^A > C_i^O$, $\varepsilon < 1$), $\frac{\partial^2\varepsilon}{\partial^2 D^{A-T}}$ would be larger than 0 ($\frac{\partial^2\varepsilon}{\partial^2 D^{A-T}} > 0$), the graph of ε is concave upward relative to D^{A-T}(Fig. 4-b); when C_i^A is smaller than C_i^O ($i.e., C_i^A < C_i^O$, $\varepsilon > 1$), $\frac{\partial^2\varepsilon}{\partial^2 D^{A-T}}$ would be smaller than 0 ($i.e., \frac{\partial^2\varepsilon}{\partial^2 D^{A-T}} < 0$), the graph of ε is concave downward (Fig. 4-d).

Notice that $\varepsilon \equiv 1$ is a critical value, which means the mass whole system unchanged and differs the evolved/altered and remained subsystem mass gain from loss relative to the initial mass of system. $D^{A-T} \equiv 1$ is also a critical value in equation (57). When $D^{A-T} > 1$, components prefer staying the evolved/altered and remained subsystem to the transported subsystem, and vice versa. Let's define components with distribution coefficient equal to 1 as **neutral mobile component**, as **the mass of such components would be evenly distributed in the evolved/altered and remained subsystem and the transported subsystem**. The concentrations in both subsystems are,

$$C_i^A = C_i^T = \frac{D_i^{A-T}}{(D_i^{A-T}-1)\varepsilon + 1} C_i^O = C_i^O, as\ D^{A-T} = 1 \quad (58)$$

Equation (58) says, no matter what evolutionary degree the system evolved, **as long as the distribution coefficients of certain components equal to 1, their concentrations in the evolved/altered and remained subsystem and transported subsystem equal their original concentrations in the initial system**. In real-word problem, we can use such property to deduce the original concentrations of components with distribution coefficients equal/close to 1, and develop other applications such as natural tracers and discrimination proxies.

Based on the knowledge proved before, we now propose the principle for selection of immobile components: **to choose the components with largest (in the form of D^{A-T}) /smallest (in the form of D^{T-A}) distribution coefficients as approximations of absolute immobile components**. Such components are called **reference (absolute) immobile components**. The following steps summarize the procedure:

a) Calculations of the ratios (i.e., the slopes) of observed compositions to the reference composition of all the samples, and plotting corresponding Isocon diagrams if feasible.
b) Clustering the ratios for each sample. Components with the same/similar distribution coefficients would form one straight line on the Isocon diagram and be classified into one group. The same group of components with different ratios indicates the samples experiencing different stages of evolution/alteration.
c) Choosing components clustered in the same group in all samples as candidate immobile components.
d) Referring to the relevant literatures on the mobility of candidate immobile components in the same or similar geological evolution processes.
e) Comparing the slope $\frac{C_i^A}{C_i^O}$ with 1.

   i) If $\frac{C_i^A}{C_i^O} > 1$ (i.e., $\varepsilon < 1$), the slope k increases as D^{A-T} increases. And thus, we choose the group with the largest slope as candidate immobile components, and choose the component with largest slope in the group as approximation of absolute immobile component.

   ii) If $\frac{C_i^A}{C_i^O} < 1$ (i.e., $\varepsilon > 1$), the slope decreases as D^{A-T} increases. Let's choose the group with the smallest slopes as candidate immobile component group, and choose the component with smallest slope in the group as approximation of absolute immobile component.

   iii) If $\frac{C_i^A}{C_i^O} \cong 1$ (i.e., $\varepsilon \cong 1$), the slope k does not change as D^{A-T} changes. This would be constant mass situation.

It is also possible to plot Isocon diagrams in the first step, but problems occur in the visualizations due to magnitudes of different components. Besides, if lots of samples collected, such as geochemical survey, plotting and analyzing Isocon diagrams would be a tedious work. It is worthy to mention that we emphasize that candidate immobile components ought to behave consistently in all samples. It is not advocated to ignore certain samples in order to get a best-fit model, unless none of the candidate component groups meet such demands. In this case, we need carefully consider dropping individual abnormal samples.

Knowledge framework of mobility

Based on the previous discussion, here we proposed a rough knowledge framework of component mobility. Component mobility is a property about components' mass partition in the evolution of system. It is a relative term, and only have meaning when specifying the concrete evolution system/process. Distribution coefficient is the dimensionless/characteristic quantity describing mobility. Absolute immobile component refers to those components of which the initial mass is conserved in the evolved/altered and remained subsystem of interest, which we can observe at present. The distribution coefficients of absolute immobile components approach positive infinity $+\infty$ (in the form of D^{A-T}) or 0 (in the form of D^{T-A}) theoretically. Absolute mobile components refer to those components of which the initial mass is conserved in the transported away/in subsystem, which possibly we are unable to observe at present. The distribution coefficients of absolute mobile components approach 0 (in the form of D^{A-T}) or positive infinity $+\infty$ (in the form

of D^{T-A}) theoretically. Absolute mobile and immobile components are the two endmembers of mobility. Between them, **partial mobile components** are defined as the initial mass of those components are conserved partially in both the evolved/altered and remained subsystem and the transported away/in subsystem. Their distribution coefficients are limited between 0 and positive infinity ($0 < D < +\infty$). "Absolute mobility" and "absolute immobility" are two relative concepts, and components absolute immobile in one subsystem are absolute mobile in the other subsystem, and vice versa. Components with distribution coefficients > 1 are compatible components, and components with distribution coefficients < 1 are incompatible components conventionally. And Components with distribution coefficients equal to 1 are **neutral mobile components**, **"neutral" means the initial mass of such components would evenly goes in the evolved/altered and remained subsystem and the transported subsystem, and their concentrations in each subsystem equal their original concentration in the initial system**. Figure 5 shows the relationships of component mobility and distribution coefficient schematically.
The Isocon analysis theory is reconstructed based on the relationship between evolved/altered and original concentrations (Eq. 39 and 40). Evolutionary degree and distribution coefficient determine their relationship in a nonlinear way together. Concepts like evolutionary degree, mass increment of system, mass increment of component, relative mass change rate of component, unit mass increment of component, relative immobile component pair, initial Isocon line, absolute Isocon line, and relative Isocon line were revised or proposed. Their exact definitions and meaning were summarized in table 1.

Application Cases

To show the knowledge demonstrated in the previous sections, we used two data sets as examples, one for forward model, and the other for inverse model.

Synthetic data

A synthetic data set was used for forward model. The data were recorded in table 2, and consisted of 8 fictive components from a to h. In this simulation, a and b were set as absolute immobile components, and c, d, e, f, g, and h were mobile elements. In addition, c and d, e and f were set as relative immobile component pairs. Two different evolutionary degree samples of A1 and A2 were used to simulate the progressive evolution stages. The evolutionary degrees of A1 and A2 were set as 1.2 and 1.5, respectively.
In order to verify the correctness of the relationship between evolved/altered concentrations and initial concentrations (i.e., Eq. 39 and 40), we calculated the theoretical concentrations after the evolution of the system based on the initial conditions by equations 39 and 40, and then compared the results with the concentrations obtained by "observation", which was simulated by calculation of the ratio of the mass of a specific component to the total mass $\frac{M_i}{M}$. The results of theoretical and observed concentrations were reported in table 3. Table 3 clearly shown the calculated theoretical concentrations are exactly the same as the observed concentrations.
To simulate the situations solving real world problem, we used the observed concentrations to inversely deduce the initial conditions of the system. First of all, three samples of origin, A1, and A2 were collected fictitiously, and their concentrations were calculated by equation $C = \frac{M_i}{M}$ as

simulation of result of chemical analysis and reported in table 3. Secondly, the standard Isocon diagrams of A1 and A2 were plotted as Fig. 6. Figure 6 showed that components a and b, c and d, and e and f formed two sets of Isocon lines, which indicates two evolution stages existed in the evolution processes. It is clearly that both absolute immobile components and all the relative immobile components fitted straight lines emitted from the origin. Furthermore, the slopes of each Isocon line were compared with each other to select the best reference immobile components. As most Isocon lines were below the initial Isocon line, assumption of the evolution degree $\varepsilon > 1$ was made. And thus, the slope k decreased as the distribution coefficient D^{A-T} increased. Therefore, we need choose the components with smallest slope as the approximation of absolute immobile component. For the convenience of comparison, the slopes were list in table 4, and a and b were easily chosen as reference immobile components. All the information of mass-transfer of other components can be calculated based on the reference frame of a and b. At last, two evolution stages were deduced by the two Isocon lines formed by a and b. Evolution degrees were calculated by $\varepsilon = \frac{1}{k_{a,b}}$, and the evolution degrees of stages A1 and A2 were 1.2 and 1.5, respectively. The results of evolution degrees calculated were the same as the values set in the beginning. Other information of interest can be deduced accordingly. It is worth noting that if we mistakenly chose components e and f as reference immobile components, we would get the wrong conclusion of mass loss of the entire system.

Real data of Riverin and Hodgson (1980)

To show how to apply the knowledge to solve real world problem, we chose a data set from a progressive altered quartz-feldspar-porphyry system (Riverin and Hodgson, 1980) as example. This data set was used by both Grant (1986) and Guo et al. (2009); therefore, it might be familiar to researchers interested in the mass-balance issue. The data set was reported in table 5, as we can see, 6 types of samples with different alteration were collected, and the fresh QF was believed to represent the original rock. The following showed the decision-making process about choice of reference immobile component.

Firstly, all the standard Isocon diagrams of each sample were plotted in Fig. 7 -a to -f. Some components formed straight lines passing the origin in all the plots. Unfortunately, it was unclear due to the magnitude problem. To tackle this problem, we divided the concentrations of each component by the corresponding mean for scaled Isocon diagrams (Fig. 7 -g to -l), and also reported the exact slope of each component in table 6. The components were classified into different groups by the slopes. It was clear that only the set of SiO_2 and Al_2O_3 clustered in one group in all samples, and consequently, they were the candidate reference immobile components. Now compare the slopes, as most of straight lines below the initial Isocon line, so assumption of $\varepsilon > 1$ was made. In this assumption, the slope k decreased as D^{A-T} increased, and thus, component with the smallest slope was the best approximation of absolute immobile component. From table 6, we knew Al_2O_3 was the best choice. Other information of interest can then be deduced based on the selected reference immobile component according to Grant (1986, 2005).

Conclusions

In this research, we discussed the essential properties of the Isocon line and built a knowledge framework of component mobility. Mobility is a relative concept. To describe the mobility of a certain component, the initial system and corresponding evolved subsystems, processes and reference frame/composition must be specified. The relationship between the final evolved/altered concentrations and the initial concentrations are determined by distribution coefficients and evolutionary degree, and equation $C_i^A = \frac{D_i^{A-T}}{(D_i^{A-T}-1)\varepsilon+1} C_i^O$ (or $C_i^A = \frac{1}{(1-D_i^{T-A})\varepsilon+D_i^{T-A}} C_i^O$ if distribution in the form of D_i^{T-A}) was proposed to express such relationship. Some new concepts were proposed, such as absolute immobile, partial immobile, and neutral immobile components. The straight lines passing the origin in the Isocon diagram reflect the relationship between evolved concentrations and original concentrations, which is determined by evolutionary degree and distribution coefficient. Components with the same/similar distributions form one straight line passing the origin. The straight lines formed by mobile components were termed relative Isocon line, which indicates the components lie on the line are relative immobile to each other. Whereas the straight lines formed by absolute immobile components were termed absolute Isocon line, which indicates the components lie on the line are absolute immobile in the evolution processes, and its slope indicates the evolutionary degree. Components experienced different evolutionary degrees would form different Isocon lines. The initial Isocon line is the reference line for all the absolute/relative Isocon lines. Absolute Isocon lines below the initial Isocon line reflect system mass gain, whereas lines above the initial Isocon line reflect system mass loss. The choice of reference immobile components is a critical step, which would matter the results of mass-transfer. The principle of choice of reference immobile components is based on the relationship between the slopes and distribution coefficients. If $\varepsilon < 1$ $(i.e.,\ C_i^A > C_i^O)$, then $\frac{\partial k}{\partial D^{A-T}} > 0$, k increases as D^{A-T} increases, and then the candidate component with largest slope is the best choice. if $\varepsilon > 1$ $(i.e.,\ C_i^A < C_i^O)$, then $\frac{\partial k}{\partial D^{A-T}} < 0$, k decreases as D^{A-T} increase, and thus the candidate component with smallest slope is the best choice. Problems still exist in the study of mass balance in the geological evolution processes, and the determination of original concentrations of parental source is a hard problem of great significance to deal with. Additionally, all the discussed knowledge are based on the assumption of homogeneous system. However, if the system is heterogeneous, how can we deal with it? Furthermore, when deciding the relationship between C^A and C^O, we simply made the decision based on the relationship of most components. However, if there are multiple groups of candidate immobile components with slopes both greater and less than 1, how should we judge the relationship between the evolutionary degree and 1?

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Figures and tables

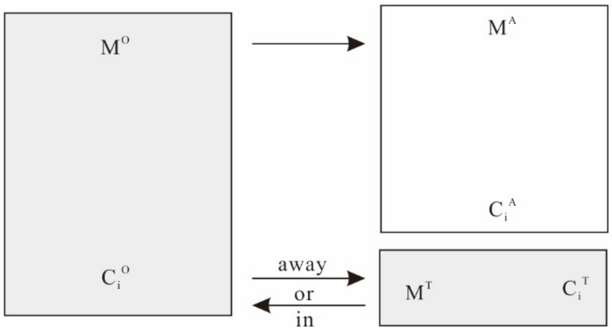

Figure 1 Schematic of the evolution system. The whole system is assumed homogeneous. The initial system consisting of different components initialized with mass of M^O and evolved with two homogeneous subsystems, one is made of materials evolved/altered and remained, and the other made of materials transported away/in. The evolved/altered and remained subsystem has mass M^A, and the transported subsystem has mass M^T. The components of interests have bulk concentrations of C^O in the initial system, C^A in the evolved/altered and remained subsystem, and C^T in the transported subsystem, respectively.

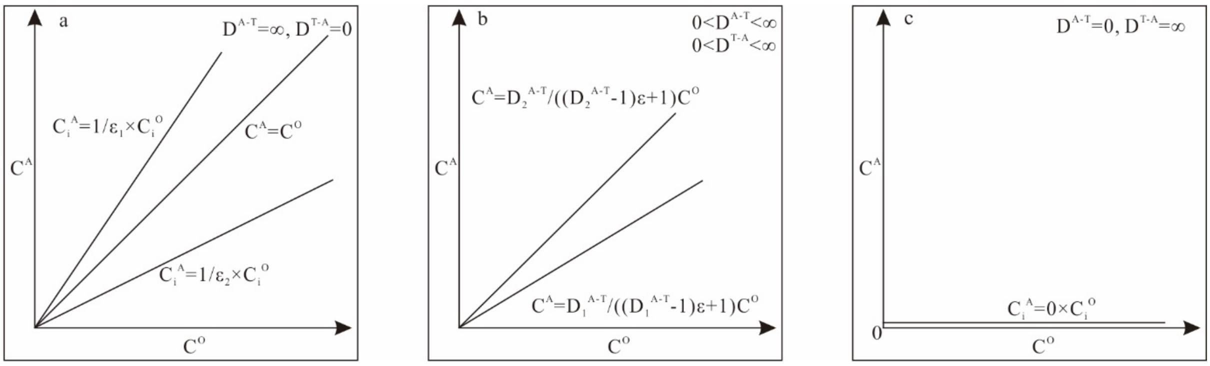

Figure 2 Schematics of Isocon line. a: Absolute immobile Isocon lines with different evolutionary degree and distribution coefficient equal to infinity. The slope reflects the evolutionary degree. Straight lines below the initial Isocon line ($C^A=C^O$) indicate the mass of the evolved/altered and remained subsystem is gained relative to the mass of the initial system, whereas lines above the initial Isocon line ($C^A=C^O$) indicate the mass of the evolved/altered and remained subsystem is lost relative to the mass of the initial system. b: Isocon lines with the same evolutionary degree and different distribution coefficients. All the components with the same/similar distribution coefficient would form one relative immobile Isocon line passing the origin and data points and are relative immobile to each other. Components with different distribution coefficients would form different relative immobile Isocon lines. c: Isocon line formed by "immobile components" in the transported subsystem. Those components have concentrations close to 0 in the evolved/altered and remained subsystem.

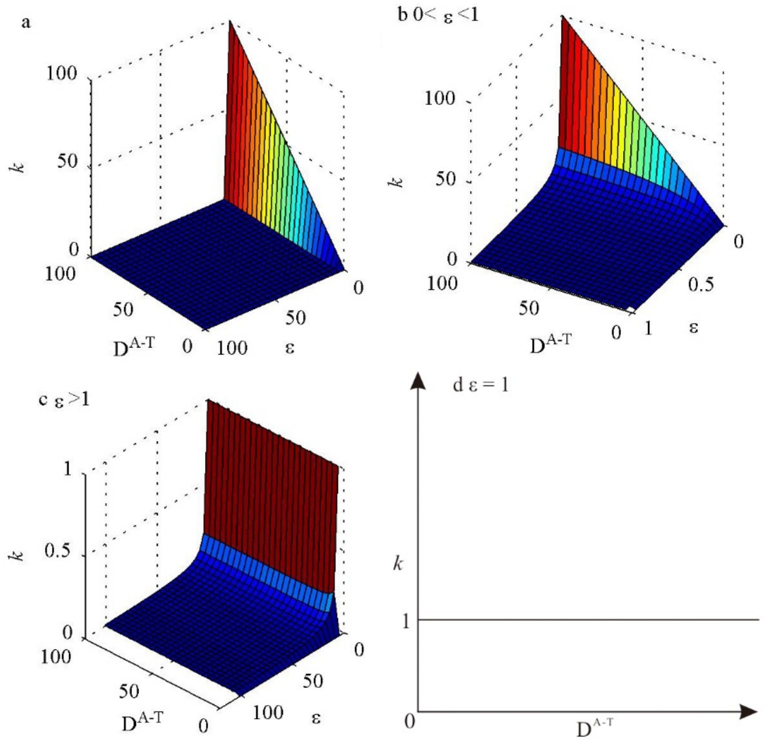

Figure 3 Schematics of the relationship among the slope, evolutionary degree, and distribution. a: the global relationship between the slope and distribution coefficient and evolutionary degree. b: the relationship between the slope and distribution coefficient as $\varepsilon < 1$. c: the relationship between the slope and distribution coefficient as $\varepsilon > 1$ d: the relationship between the slope and distribution coefficient as $\varepsilon = 1$.

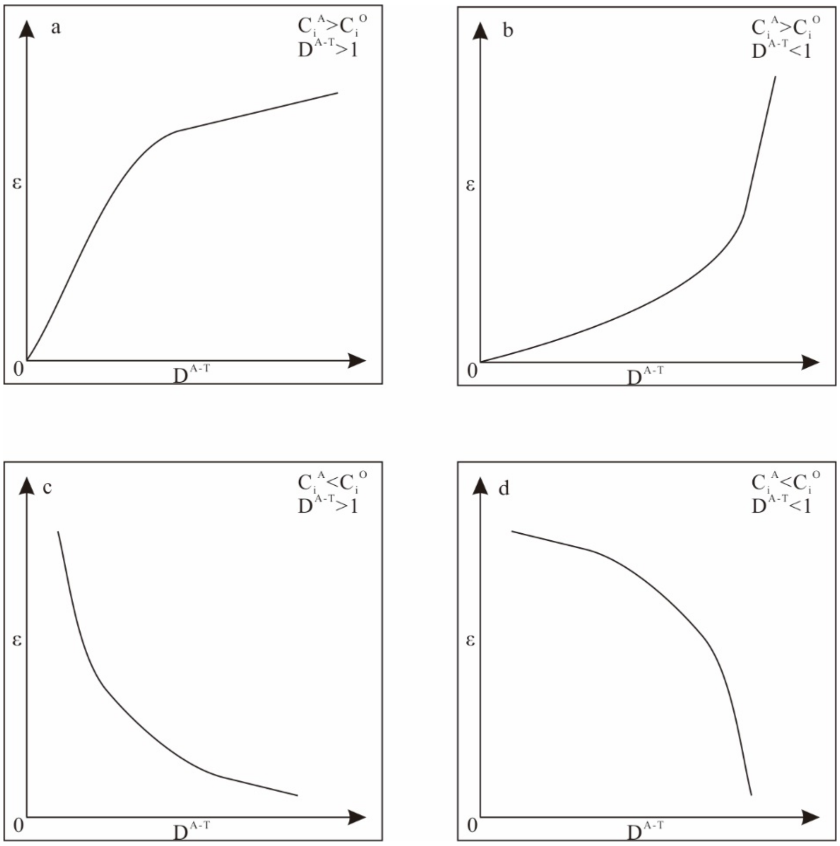

Figure 4 the relationship between evolutionary degree ε and distribution coefficient $D^{A\text{-}T}$. a: When $C_i^A > C_i^O$ $(i.e.,\ \varepsilon < 1)$ and $D^{A-T} > 1$, then $\frac{\partial \varepsilon}{\partial D^{A-T}} > 0$ and $\frac{\partial^2 \varepsilon}{\partial^2 D^{A-T}} < 0$, and thus ε increases as D^{A-T} increases and the graph of ε relative to $D^{A\text{-}T}$ is concave upward. b: When $C_i^A > C_i^O$ $(i.e.,\ \varepsilon < 1)$ and $D^{A-T} < 1$, then $\frac{\partial \varepsilon}{\partial D^{A-T}} > 0$ and $\frac{\partial^2 \varepsilon}{\partial^2 D^{A-T}} > 0$, and thus ε increases as D^{A-T} increases and the graph of ε relative to $D^{A\text{-}T}$ is concave downward. c: When $C_i^A < C_i^O$ $(i.e.,\ \varepsilon > 1)$ and $D^{A-T} > 1$, then $\frac{\partial \varepsilon}{\partial D^{A-T}} < 0$ and $\frac{\partial^2 \varepsilon}{\partial^2 D^{A-T}} > 0$, and thus ε decreases as D^{A-T} increases and the graph of ε relative to $D^{A\text{-}T}$ is concave upward. d: When $C_i^A < C_i^O$ $(i.e.,\ \varepsilon > 1)$ and $D^{A-T} < 1$, then $\frac{\partial \varepsilon}{\partial D^{A-T}} < 0$ and $\frac{\partial^2 \varepsilon}{\partial^2 D^{A-T}} < 0$, and thus ε decreases as D^{A-T} increases and the graph of ε relative to $D^{A\text{-}T}$ is concave downward.

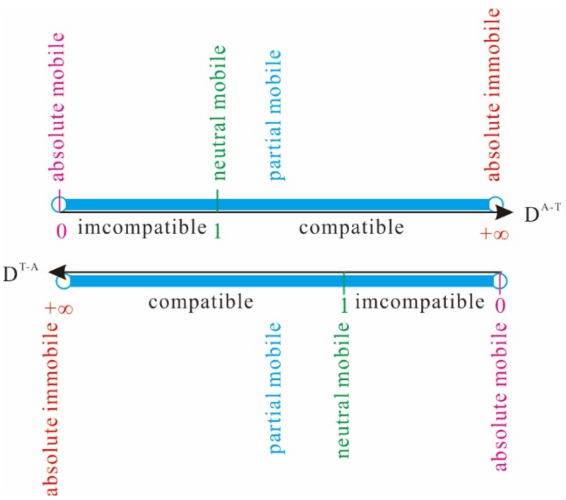

Figure 5 Schematic of relationship between component mobility and distribution coefficient. It reflects the "mobile" and "immobile" are relative concepts related to distribution coefficient. Absolute immobile and mobile are two endmembers in the mobility property. Between them, "partial mobile" describes components with 0< distribution coefficients <∞, which contains conventional compatible and incompatible components.

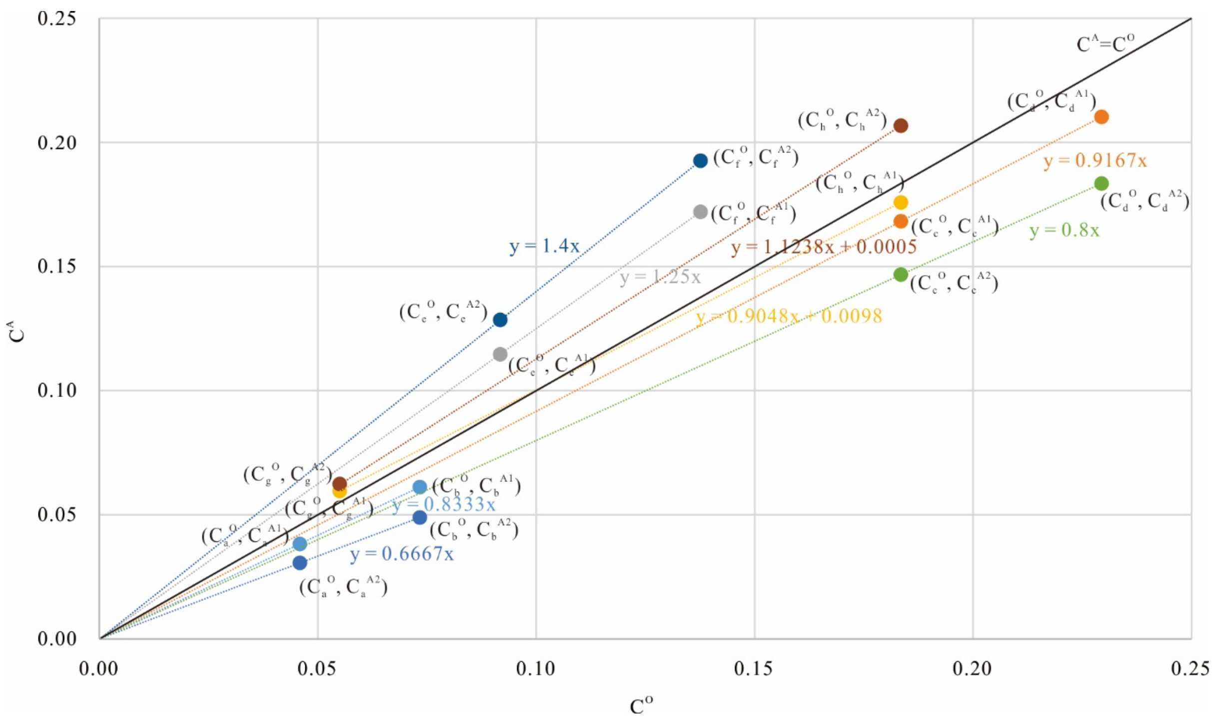

Figure 6 The standard Isocon diagram of synthetic data set. The solid line is the initial Isocon line. Each pair of a and b, c and d, and e and f forms two Isocon lines. The two Isocon line formed by a and b are absolute immobile Isocon lines, and their slopes reflect the evolutionary degrees. The Isocon lines formed by c and d, and e and f are relative immobile Isocon lines, and the components lying on them are relative immobile to each other but mobile relative to the system. Components with the same/similar distribution coefficients form one straight line (i.e., Isocon line) connecting the origin and data points.

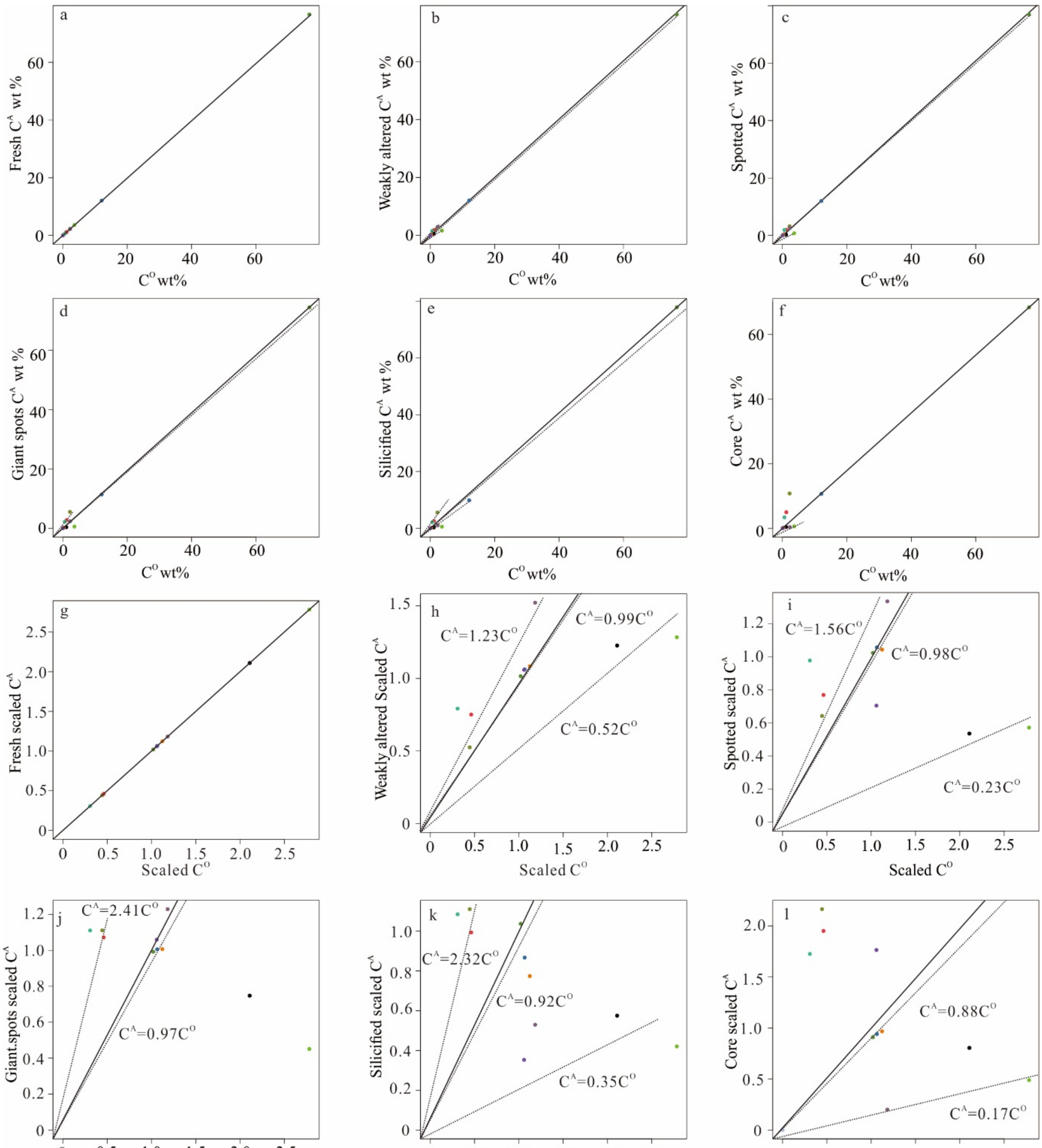

Figure 7 The Isocon diagrams of real data set from Riverin and Hodgson (1980). a-f: the standard Isocon diagrams of each type sample, visualization problem occurs in these plots due to magnitude issue. g-l: the Isocon diagrams of each type sample scaled by the mean. The solid line is the initial Isocon line. It is clear that SiO_2 and Al_2O_3 formed one Isocon line in all types of samples. Both the standard Isocon diagrams and scaled Isocon diagrams presented a progressive alteration process.

Table 1 Some revised/proposed concepts and definitions of mobility and Isocon method

Concept	**Definition**	**Symbol**
System evolution degree	The ratio of the mass of the evolved and remained subsystem to the mass of initial system	ε
Distribution/partition coefficient	The ratio of component concentrations in the two corresponding subsystems	D
Absolute immobile component	Component with distribution coefficient equal to positive infinity	-
Absolute mobile component	Component with distribution coefficient equal to 0	-
Neutral mobile component	Component with distribution coefficient equal to 1	-
Partial mobile component	Component with distribution coefficient between 0 and 1	-
Relative immobile component pair	Components with the same/similar distribution coefficients	-
Mass increment of the system	The mass difference between the evolved/altered subsystem and the initial system	ΔM
Mass increment of component	The difference between the mass of component i in the evolved/altered and remained subsystem and initial system	ΔM_i
Unit mass increment of component	The ratio of the mass increment of component to the mass of initial system	ΔC_i
Relative mass change rate of the system	The ratio of the mass increment of evolved/altered and remained subsystem to the mass of initial system	λ
Relative mass change rate of component	The ratio of the mass increment of component i to its original mass	λ_i
Initial Isocon line	The Isocon formed by component original concentrations against component original concentrations	-
Absolute Isocon line	The Isocon formed by component with distribution coefficient equal to infinity	-
Relative Isocon line	The Isocon formed by component with the same/similar distribution coefficient	-
Slope	The ratio between the evolved/altered concentrations and (reference) original concentrations	k
Reference composition	The composition serves as approximation of the original composition when the real original composition unknown	C^O
Original composition	The real concentrations in the parental sources	C^O
Reference absolute immobile component	The component serves as approximation of the absolute immobile component	-

Table 2 The synthetic data and initial conditions

Item	a	b	c	d	e	f	g	h	Total
ε1	1.20								
ε2	1.50								
$D_i^{A\text{-}T1}$	∞	∞	1.83	1.83	0.50	0.50	0.72	1.28	
$Di^{A\text{-}T2}$	∞	∞	2.00	2.00	0.64	0.64	0.81	0.82	
$D_i^{T\text{-}A1}$	0.00	0.00	0.55	0.55	2.00	2.00	1.38	0.78	
$Di^{T\text{-}A2}$	0.00	0.00	0.50	0.50	1.57	1.57	1.24	1.22	
M_i^O (Kg)	5.00	8.00	20.00	25.00	10.00	15.00	6.00	20.00	109.00
M_i^{A1} (Kg)	5.00	8.00	22.00	27.50	15.00	22.50	7.80	23.00	130.80
M_i^{A2} (Kg)	5.00	8.00	24.00	30.00	21.00	31.50	10.20	33.80	163.50
ΔM_i^{A1} (Kg)	0.00	0.00	2.00	2.50	5.00	7.50	1.80	3.00	21.80
ΔM_i^{A2} (Kg)	0.00	0.00	4.00	5.00	11.00	16.50	4.20	13.80	54.50

Table 3 Concentrations calculated by equations 39 and 40 and $\frac{M_i}{M}$

Method	Item	a	b	c	d	e	f	g	h	Total
M_i/M	C_i^O %	4.59	7.34	18.35	22.94	9.17	13.76	5.50	18.35	100.00
	C_i^{A1} %	3.82	6.12	16.82	21.02	11.47	17.20	5.96	17.58	100.00
	C_i^{A2} %	3.06	4.89	14.68	18.35	12.84	19.27	6.24	20.67	100.00
Equations 39 and 40	C_i^{A1} %	3.82	6.12	16.82	21.02	11.47	17.20	5.96	17.58	100.00
	C_i^{A2} %	3.06	4.89	14.68	18.35	12.84	19.27	6.24	20.67	100.00

Table 4 The slopes of the synthetic data

Item	a	b	c	d	e	f	g	h
k_{A1}	0.8333	0.8333	0.9167	0.9167	1.2500	1.2500	1.0833	0.9583
k_{A2}	0.6667	0.6667	0.8000	0.8000	1.4000	1.4000	1.1333	1.1267

Table 5 The original and scaled QFP data from Riverin and Hodgson (1980)

Item	SiO_2	Al_2O_3	FeO	CaO	MgO	K_2O	Na_2O	TiO_2	P_2O_5	H_2O
Fresh	76.56	12.08	2.22	1.10	1.18	2.30	3.64	0.29	0.03	0.61
Weakly altered	76.23	12.06	2.62	0.64	1.92	2.96	1.68	0.28	0.03	1.57
Spotted	76.96	12.01	3.21	0.28	1.97	2.60	0.75	0.27	0.02	1.94
Giant spots	74.47	11.41	5.54	0.39	2.74	2.39	0.59	0.26	0.03	2.20
Silicified	77.84	9.84	5.54	0.30	2.54	1.03	0.55	0.20	0.01	2.15

Core	68.36	10.68	10.80	0.42	4.99	0.39	0.64	0.25	0.05	3.42
Mean	75.07	11.35	4.99	0.52	2.56	1.95	1.31	0.26	0.03	1.98
Scaled Fresh	1.02	1.06	0.45	2.11	0.46	1.18	2.78	1.12	1.06	0.31
Scaled Weakly altered	1.02	1.06	0.53	1.23	0.75	1.52	1.28	1.08	1.06	0.79
Scaled Spotted	1.03	1.06	0.64	0.54	0.77	1.34	0.57	1.05	0.71	0.98
Scaled Giant spots	0.99	1.01	1.11	0.75	1.07	1.23	0.45	1.01	1.06	1.11
Scaled Silicified	1.04	0.87	1.11	0.58	0.99	0.53	0.42	0.77	0.35	1.08
Scaled Core	0.91	0.94	2.17	0.81	1.95	0.20	0.49	0.97	1.76	1.73

Table 6 The slopes $\frac{C_i^A}{C_i^O}$ of QFP data from Riverin and Hodgson (1980)

Item	Fresh	Weakly altered	Spotted	Giant spots	Silicified	Core
H_2O	1	2.5738	3.1803	3.6066	3.5246	5.6066
MgO	1	1.6271	1.6695	2.3220	2.1525	4.2288
K_2O	1	1.2870	1.1304	1.0391	0.4478	0.1696
FeO	1	1.1802	1.4459	2.4955	2.4955	4.8649
P_2O_5	1	1.0000	0.6667	1.0000	0.3333	1.6667
Al_2O_3	1	**0.9983**	**0.9942**	**0.9445**	**0.8146**	**0.8841**
SiO_2	1	**0.9957**	**1.0052**	**0.9727**	**1.0167**	**0.8929**
TiO_2	1	0.9655	0.9310	0.8966	0.6897	0.8621
CaO	1	0.5818	0.2545	0.3545	0.2727	0.3818
Na_2O	1	0.4615	0.2060	0.1621	0.1511	0.1758