

VOLUME 2

# Hydrogeochemistry Fundamentals and Advances

Mass Transfer and  
Mass Transport

Viatcheslav V. Tikhomirov

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## Volume 2: Mass Transfer and Mass Transport

Viatcheslav V. Tikhomirov



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## Abstract

This book is the second part of a course, "Fundamentals of Hydrogeochemistry." It reviews spontaneous processes responsible for the formation of ground water composition and properties. It includes four major sections. The first section introduces the basics of thermodynamics and provides the concept of properties of chemical reactions. The second section is devoted to basic processes of the formation of natural waters properties and composition in the geological environment. The main attention is devoted to the water mass exchange with rock, subsurface gas, non-polar liquids and biochemical processes. The third section reviews processes of mass-transfer in the geological medium. In the fourth section methods of hydrogeochemical forecasting are described.

The textbook is intended for students specializing in geology, geochemistry, hydrogeology and ecology, and also may be of use to hydrologists and oceanologists.

*Reviewer*

*Doctor of Geology, Prof. M.V. Charykova (S.-Petersb. State Univ.)*

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of the Sankt-Petersburg State University*

## Preface

This book is part II of a textbook *Fundamentals of Hydrogeochemistry*, part I of which was published in 2012. Whereas part I dealt with methods of study and description of the hydrochemical state of the geological medium, part II mostly touches upon spontaneous processes, which occur in ground waters. The processes are studied in consideration of the complexity of the geological environment in order to give an idea of their numerical modeling methods. In this connection the book contains four main sections.

Chapter one gives general ideas of the water solution's thermodynamical state and spontaneous reactions in it, their laws, energy, direction and kinetics.

Chapter two reviews main processes of spontaneous formation composition of ground water as an aggregate of many similar reactions between a multitude of components in the water composition. In this connection is introduced a concept of homogenous processes (redox, acid-base, complex formation, etc.) and mass exchange between water and rock, subsurface gas and non-polar liquids (ion exchange, surface complex formation, dissolution and mineral formation, physical absorption, etc.), as well as of biochemical and isotope processes.

Chapter three is about the element or compounds migration in the process of mixing and flow of ground water.

And lastly, chapter four gives an idea of hydrogeochemical forecasting and modeling methods.

The publication of this textbook was made due to the help by P.K. Konasavsky, A.A. Potapov and M. Gorfunkel who took upon themselves the ungrateful labor of reading the manuscript and gave helpful advice.

The author will appreciate any comments and advice about the textbook content and requests that comments be sent to:

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# Spontaneous Processes and Mineral Equilibrium

No density or weight and no size.  
They are just functions of varying rate.  
All in existence due to pressure delta,  
Temperature, mass, potential.  
The stream of time is terribly uneven,  
The space is just variety of shapes.  
There is not one but many mathematics...  
*Maximilian Voloshin. Cosmos (1923)*

Evolution of properties and composition in the geological medium is first of all change in properties and composition of ground water as a result of their reaction to the action of external factors. Cosmic, climatic, hydrological, biology-soil, anthropogenic and other factors disrupt both energy and material equilibrium of the medium, and the medium's resistance to this action and tendency to restore the equilibrium are the substance of *spontaneous processes* subordinated only to the laws of thermodynamics, physics and chemistry.

Before reviewing spontaneous processes, we must have a concept of the laws of thermodynamics, physics and chemistry, which control them. At the base of hydrogeochemical processes are the multitude of elements in the composition of water solutions and chemical reactions between them. For this reason familiarity with processes should begin with familiarity with the laws of conversion of one substance in the water composition into another one.

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# 1

## Chemical Reactions

Ground water, thermodynamically, is part of a complex heterogeneous system called the geological medium. This medium includes, beside ground water, rocks and often also underground gas or complex non-polar liquids (oil, oil products, etc.).

Rocks as aggregate of various minerals compose the largest part of the geological medium. Each mineral may be considered as an individual solid phase of the phase of constant composition. Minerals may be solid solutions and may contain substitutional impurities, which affect their chemical properties. However, hydrogeochemists more often ascribe to them permanent composition. This allows minerals to be viewed as elements of a single compound  $i$  with a molar fraction  $C_i = 1$ . The presence of impurities is usually ignored.

Ground water in its substance is a mixture of micro-particles of various size and composition poorly bonded between themselves. In terms of size these particles are drastically dominated by molecular size (less  $1\text{ nm}$ ), which in aggregate form **real solution**. In smaller amounts are present uniformly distributed micelles ( $1$  to  $100\text{ nm}$ ). With the growth of their content the solution becomes colloid solution (sols), and sometimes even forms gels. Even larger particles (greater than  $100\text{ nm}$ ) form

suspensions and emulsions. Poly-molecular particles of similar properties and composition (for instance, all grains of the same mineral, gas bubbles or liquid drops) may be considered as individual homogenous substances: minerals, non-polar liquids or underground gases. In such case it is convenient to merge suspended mineral particles and enclosing rock into one medium. Lastly, ground water may be treated also as a live **ecosystem**. The aggregate of its live organisms (plants, animals, micro-organisms and fungi) form **biocenose**, which defines the nature of biochemical processes and plays an important role in the formation and its composition.

Overall liquid ground water is also a complex heterogeneous system, in which should be discerned: 1) real solution; 2) inert suspended substance; 3) biocenose (live dispersed matter).

## 1.1 Real Water Solution

Real solutions where individual components are visually indistinguishable compose most of the ground water volume and define its properties and composition. As a rule, it is identified with ground water in hydrogeochemistry studies.

Properties and composition parameters of this solution are called **thermodynamic state parameters**. They are subdivided into extensive and intensive ones. The **extensive** parameters include those which depend on the size of the medium or system, are proportionate with them and, therefore, are additive. Such are mass –  $m$ , volume –  $V$ , amount of the matter, heat, energy, etc. The **intensive** parameters include parameters, whose value does not depend on the size of the system or phase, namely, pressure –  $P$ , temperature –  $T$ , density –  $d$ , concentration –  $C$ , etc. They reflect change in the state of water.

Extensive and intensive parameters are tied between themselves. Change in any of them results in changes in the other ones. The ideas of cause and effect interrelation between these parameters define the **model of solution state**, and the mathematical expression of a given interrelation is the **equation of state of the solution**. It is sufficient to know some minimum number of its parameters for the complete description of the solution properties. As a rule, as such parameters of state serve first of all most easily measured, namely: volume, pressure, temperature and composition ( $V, P, T, C_i$ ). Equations of state for the complex solutions are constructed based on equations of state of pure substances, which make its composition. For this are needed additional parameters, associated with the mixing

processes (mixing proportions, interaction coefficients, etc.). Parameter values and their interrelation are determined both theoretically, i.e., according to logic, and experimentally. For this reason, equations of state for the solutions, as a rule, include semi-empirical functional interrelations.

### 1.1.1 Properties of Water Solution

Solutions have special properties, which identify them among other substances. Real water solution is no exception.

1. First of all, it has variable composition, and the concentration of its substances are not constant.  $H_2O$ , as the dominant substance – solvent has most stable concentration, the others are present as admixtures. Their content varies within a very wide range and is usually quoted in values of concentration (molarity, molality, molar fraction, etc.).
2. Any solution is a medium with ***distributed parameters***. This means that within its limits composition and properties may change, but gradually. For this reason, specific stable boundaries between the waters of different composition are absent. On the contrary, concentration and property changes within the space coordinate of a single solution display gradients, i.e., values of parameter changes attributed to a unit of distance.
3. Real water solutions are capable of mixing with one another in unlimited proportions. At mixing, their extensive parameters are summed up whereas the intensive ones are levelling off.

If we treat mixing of different water solutions as a purely physical process, with no consideration of their chemical interaction, the mixture composition may be easily calculated.

Let us assume that mixed are only two solutions with salinities  $m_0$  and  $m_1$  and concentrations of component  $i$  respectively  $C_{0,i}$  and  $C_{1,i}$ . If the fraction of one of them in unit volume of the mixture is equal to  $\alpha$ , then the corresponding fraction of the other one will be equal to  $1 - \alpha$ , a salinity and concentration of the component  $i$  in the mixture will be the sum of the two addends:

$$m = \alpha \cdot m_0 + (1 - \alpha) \cdot m_1, \quad (1.1)$$

$$C_i = \alpha \cdot C_{i,0} + (1 - \alpha) \cdot C_{i,1}. \quad (1.2)$$

If mixed are two waters with known content of the component  $i$ , which does not enter chemical interaction, then from the composition of the mixture it is possible to determine proportions of the mixed waters:

$$\alpha = \frac{C_i - C_{i,1}}{C_{i,0} - C_{i,1}} \quad (1.3)$$

The value  $\alpha$ , which may range between 0 and 1, is often called **fractional mixture concentration**. If the component  $i$  is not present in one of mixed waters ( $C_{i,1} = 0$ ), the fractional concentration is equal to the ratio  $C_i/C_{i,0}$ .

To determine the fractional concentration of mixing are used, as a rule, strong acids or bases, which poorly form insoluble salt. For instance, to study the fraction of sea or fresh water in their mixture are used  $\text{Cl}^-$  or  $\text{Na}^+$  but not sulphates, varbonates,  $\text{Ca}^{2+}$  or  $\text{Mg}^{2+}$ . In particular, the fraction of sea water in such mixture is determined from the following equation:

$$\alpha_{\text{sea}} = \frac{C_{\text{water,Cl}} - C_{\text{water,Cl,fresh}}}{C_{\text{water,Cl,sea}} - C_{\text{water,Cl,fresh}}} \quad (1.4)$$

where  $C_{\text{water,Cl}}$ ,  $C_{\text{water,Cl,sea}}$  and  $C_{\text{water,Cl,fresh}}$  are weight contents of  $\text{Cl}^-$ , correspondingly, in mixtures, sea and fresh waters. If the chlorine content in fresh water is negligibly low and may be disregarded ( $C_{\text{water,Cl,fresh}} \approx 0$ ), then

$$\alpha_{\text{sea}} = 0.00177 \cdot C_{M,\text{Cl}} \quad (1.5)$$

where  $C_{M,\text{Cl}}$  is  $\text{Cl}^-$  concentration in millimoles per 1 liter.

In the absence of chemical interaction value  $\alpha_i$  does not depend on the nature of the component. That is why the mixture composition may be calculated if the composition's mixed solutions are known. For this it is necessary to equate Equations (1.4) for two different components (or one component  $i$  and salinity) and to unfold the obtained equation as a function of interrelation between their concentrations in the mixture:

$$C_i = m \frac{(C_{i,1} - C_{i,2})}{m_1 - m_2} + \frac{m_1 \cdot C_{i,2} - m_2 \cdot C_{i,1}}{m_1 - m_2}. \quad (1.6)$$

Equation (1.6) shows that at mixing of two waters concentration of their components, which do not take part in chemical reactions are not removed from the solution, are tied between themselves in direct linear relation. For this reason the discovery of such linear interrelation in the ground water composition may indicate the participation in their formation of the mixing process.

4. All solution parameters are tied between themselves by the equation of state. The most important component of such an equation is the connection between intensive and extensive parameters. This interrelation has a complex, not fully studied nature. However, it noticeably simplifies and is amenable to experimental studies in ideal double-component solutions with dominance of one component – solvent.

For characterization of the interrelation between the composition and extensive properties of the solution the outstanding American physico-chemist Gilbert Newton Lewis (1875–1946) introduced additional intensive parameters under the common name **partial molar quantity**. Among them are partial molar volume, partial molar heat capacity, chemical potential, *etc.*

If we add to a water solution  $\Delta N_i$  moles of any component  $i$ , its volume, heat, energy and other extensive properties will change by some value  $\Delta g$ . Such change of an extensive parameter, related to one mole solved component  $i$ , is called **mean partial quantity**

$$\bar{g}_i = \left( \frac{\Delta g_i}{\Delta N_i} \right)_{P, T, N_1, N_2, \dots, N_k}, \quad (1.7)$$

where  $\bar{g}_i$  is mean partial molar value of any extensive property, for instance volume ( $\text{cm}^3 \cdot \text{mole}^{-1}$ ) or heat capacity ( $\text{cal} \cdot \text{mole}^{-1} \cdot \text{deg}^{-1}$ ). It depends on concentration. That is why the derivative of this interrelation should be considered:

$$\bar{g}_i = \left( \frac{\partial g_i}{\partial N_i} \right)_{P, T, N_1, N_2, \dots, N_k}, \quad (1.8)$$

Which characterized real partial molar values. Thus, **true partial quantity** of a component  $i$  is partial derivative of any extensive property of its ideal solution ( $g_i$ ) over its concentration at constant temperature and pressure.

The partial molar values per se are intensive properties as they do not depend on the total amount of solution and may be both positive and negative. If the solution pressure and temperature do not change, any of its extensive property is a function only of its composition:

$$g = f(N_1, N_2, N_3, \dots, N_k).$$

Let us assume that to a solution are added sequentially all its components by infinitely small amounts at constant pressure and temperature. At

each addition any extensive parameter changes by values  $\partial g_1, \partial g_2, \dots \partial g_k$ , which respectively are equal:

$$\partial g_1 = g_1 \partial N_1, \partial g_2 = g_2 \partial N_2, \dots \partial g_k = g_k \partial N_k. \quad (1.9)$$

In which case the derivative of the change of any extensive property at the addition of one component  $i$  may be represented as the sum of two addends:

$$\partial g_i = g_i \partial N_i + N_i \partial g_i, \quad (1.10)$$

And at the addition of all components total value of the extensive properties  $G$  will change by

$$\partial G = \sum g_i \partial N_i + \sum N_i \partial g_i. \quad (1.11)$$

If the amounts  $\partial N_1, \partial N_2, \partial N_3, \dots, \partial N_k$  have the same proportions as in the initial solution, the composition of the latter does not change. This is the same as mixing two solutions of the same composition: the solution amount increases, and its composition does not. In this case the very partial molar values  $g_i$  also do not change, and  $\sum N_i \partial g_i$  in the second addend in Equation (1.11) are equal to 0. Then

$$\partial G = \sum g_i \partial N_i. \quad (1.12)$$

Integrating Equation (1.12), on condition of constancy median partial molar values  $\bar{g}_i$  we obtain Equation

$$G = \sum_{i=1} \bar{g}_i N_i, \quad (1.13)$$

Which is called the **first Gibbs-Duhem equation**. It shows that any extensive property  $g$ , for instance volume, heat capacity or energy of the solution, may be determined from its composition, if corresponding median partial molar values of its components are known. For instance, if the mole amount of individual components in the composition of a solution and their partial molar volumes are known, then the volume of the entire solution will be equal to the sum of their products.

At the addition of not all components or all but in other proportions, the composition of the source solution noticeably changes, but the addend in the equation (1.11)  $\sum N_i \partial g_i \neq 0$ . Equating equations (1.11) and (1.12), we obtain **the second Gibbs-Duhem Equation**:

$$\sum N_i \partial g_i = 0 \quad (1.14)$$



It describes the association between partial molar values of different components in one solution at constant temperature and pressure. It follows from it that if content of only one component changes, the partial molar values of all components change, but so that

$$N_i \left( \frac{\partial g_1}{\partial N_1} \right)_{P,T,N_i} = - \left[ N_2 \left( \frac{\partial g_2}{\partial N_1} \right)_{P,T,N_i} + N_3 \left( \frac{\partial g_3}{\partial N_1} \right)_{P,T,N_i} + \dots + N_k \left( \frac{\partial g_k}{\partial N_1} \right)_{P,T,N_i} \right]. \quad (1.15)$$

In other words, an increase in an extensive parameter of a solution due to addition of a component  $i$  is compensated by a decrease of median partial molar values of the remaining components in its composition.

If both parts of Gibbs-Duhem equation is divided by  $\sum N_i$ , i.e., if they are related to 1 mole of the solution, the equations (1.13) and (1.14) will assume the form:

$$G_M = \sum_{i=1} \bar{g}_i C_i, \quad (1.16)$$

$$\sum_{i=1} C_i \partial g_i = 0, \quad (1.17)$$

where  $G_M$  is median extensive parameter (volume, mass, heat capacity, etc.) of 1 mole of the solution.

Equations (1.13), (1.14), (1.16) and (1.17) are very important for further understanding of the effect of change in water composition of solutions on their extensive properties, first of all on volume and energy. In this connection very significant are median partial molar values of the components in water solutions, which are determined experimentally in pure solutions of individual components at an increase of concentration by 1 mole. The obtained results may be found in reference literature (Naumov *et al.*, 1971; Wagman *et al.*, 1982; CRC Handbook of Chemistry and Physics, 2004–2005, etc.).

### 1.1.2 Composition of Water Solution

Real composition of ground water is much more complex than the analytical one. It is a whole and very brittle formation created by the forces of