Metallogenic material accumulation simulation in diffusion-reaction system

Chen Ming \textsuperscript{a}, Yu Chongwen \textsuperscript{b}, Yan Guangsheng \textsuperscript{c}, Cheng Qiuming \textsuperscript{d}, Liu Xiaoduan \textsuperscript{e}

\textit{a.} Research Center of Bioenvironmental Geochemistry, Chinese Academy of Geology Sciences, Beijing, China, 100037. hcenming@public3.bta.net.cn

\textit{b.} Institute of geochemistry, Faculty of geology, China University of Geosciences, Beijing, China, 100083. yuchongw@public.bta.net.cn

\textit{c.} Research & Development Center, China Geological Survey, Land and Mineral Resource Ministry, Beijing, China, 100083, yguangsheng@mail.cgs.gov.cn

\textit{d.} Department of Earth and Atmospheric Science/Department of Geography Faculty of Pure and Applied Science, York University, Toronto, Canada, qiuming@yorku.ca

\textit{e.} Research Center of Bioenvironmental Geochemistry, Chinese Academy of Geology Sciences, Beijing, China, 100037. ebegclxd@public3.bta.net.cn

\textbf{ABSTRACT} Hydrothermal mineralization is one of the most important types of metal accumulation. Diffusion-reaction system, \( \frac{\partial C}{\partial t} = F(C) + \varepsilon \frac{\partial^2 C}{\partial x^2} \), is a typical hydrothermal metallogenetic system and plays an important role in research of metallogenic processing. “Coupled map lattices” is used to study the common characteristics of diffusion-reaction systems. Frequently observed in wild sites and mining stopes, the features of hydrothermal deposit are commonly seen in metamorphic, magmatic and sedimentary ore deposits. According to the theory of stability of non-linearity science, the mineralisation occurring in diffusion-reaction systems is described as a quantum process. Bifurcation manifests as spatio-temporal fractality in the structure of the system, bifurcation is not only an integral behavior of the system, but also, with the developing of the system, forced the ore-forming element to be at some certain states in the hydrothermal liquid. If the content of a component is greater than the fixed point, \( C^* \), at time \( t \) and

\footnotesize{\textsuperscript{1} This paper is financially supported by the Natural Science Fund of China. Contract code: 49973015}
node $i$, $C_t(i)$, then $C_{t+1}(i)$ may less than $C^*$ at time $t+1$. Alternative state oscillation of the variable may causes precipitation of or-forming element, and therefore becomes an important part of the related metallogenic process. When the bifurcation occurs downwards, the excrescent material is forced to solidify; when it occurs upwards, ore-forming material is not enough in the fluid and has to dip out from somewhere. The integral irreversibility of metallogenic system illuminates this kind of dipping is possible, and the higher activity of ions in liquid (than in solid mineral grain) provides an advantageous condition.

The spectra of the Lyapunov exponents in the entirety of parametric space of the system are prepared. Bifurcation is not only an integral behavior of the system. The fluctuation of the content of the metal in liquid phase presents that the content of ore-forming material in fluid will be forced to be at certain values. This is a possible mechanism by which the ore-forming material is pumped from the environment media and precipitated to form solid mineral crystals. The concentration of the material will reach its maximum at the edge of chaos. This may imply a special mechanism of the formalization of ore deposit. Ore bodies, ore deposits and metallogenetic district may be at the edge of chaos.

**Keyword** hydrothermal metallogenic system, diffusion-reaction system, ore-forming process, edge of chaos, complexity, computer simulation

### 1 Introduction

Field geology experiments show that characteristics of fluid kinetics can be observed almost in all kind of mineral resource. Cumulation procedure of a metallogenetic element is coupled of flowing, diffusion and reaction procedures in hydrothermal fluid. Diffusion-reaction system (D-R system) is commonly seen in metamorphic, igneous and sedimentary metallogenetic processes. The results of computer simulation are thus of generalization.

D-R system can be simulated by means of “coupled map lattices”(K. Kaneko, 1984; 1989). Its evolvement in even medium can be written (Badii, R. & Politi, A. 1997; Bak, P. & Paczuski M. 1996) as

$$\frac{\partial C}{\partial t} = F(C) + D \frac{\partial^2 C}{\partial x^2} + \epsilon \frac{\partial^3 C}{\partial x^3},$$

where $\frac{\partial C}{\partial t}$ is the concentration of a metal $C$ evolving with time $t$; $F(C)$ is a reaction function;
\( D \frac{\partial^2(C)}{\partial x^2} \) is the item of flow; \( \varepsilon \frac{\partial^2(C)}{\partial x^2} \) is the item of diffusion. J.T. Yiyama, K. Suzuki and M. Akaogi et al (1990) used this model to simulate the material transfer during metamorphic processes.

This model was also used to simulation metal metallogenic process (Chen Ming, 2000). Three extremities are found with the variety of the two parameters \((\alpha, \varepsilon)\). The standard cumulated concentration of metallogenic metal can be estimated. According to the simulation, metallogenic materials assemble to the peak while the system be at the state of edge of chaos (Yu, 1998; Tel, 1990). Research of metallogeny of the deposits in Yangtze Craton also proved that “large ore deposits and metallogenic districts at the edge of chaos” (Yu Chongwen, 1999). This provides an important clue for mineral resource exploration.

### 2 D-R system and its simulation

Divide a one-dimensional geological medium, of which the length is \( N \), into \( N \) sections. The sequence numbers are \( 1, 2, \ldots, N, N+1 \). Under periodic condition, node 1 equals node \( N+1 \), meaning \( C(1) = C(N+1) \). The reaction item can be written as a nonlinear projection function (Turcotte, 1992; K. Kaneko, 1984; 1989)

\[
C(i) \rightarrow C(i) = F[C(i)].
\] (2)

By means of coupled map lattices, formula (1) can be discrete to

\[
C_{i+1}(i) = F[C(i)] + \frac{\varepsilon}{2} [F[\varepsilon (i+1)C(i+1)] - 2F[\varepsilon (i)C(i)] + F[\varepsilon (i-1)C(i-1)]]
\] (3)

Generally, \( F(x) \) is presented as the Logistic function to study the behavior of D-R system (J.T. Yiyama, K. Suzuki, M. Akaogi, et al, 1990; Turcotte, 1992; K. Kaneko, 1989)

\[
F(C) = 1 - \alpha C^2,
\] (4)

Where \( \alpha \) is the bifurcation parameter. Thus formula (4) becomes

\[
C_{i+1}(i) = F[C(i)] + F[\varepsilon (i+1)C(i+1)] - 2F[\varepsilon (i)C(i)] + F[\varepsilon (i-1)C(i-1)]
\]
Formula (5) is an iteration function containing parameters of space \( i \) and time \( t \). One time of iteration represents one step of evolution of the system. The ranges of \( \alpha \) and \( \epsilon \) are \([0, 1]\) and \([0, 2]\) respectively. The system collapses when \( \epsilon > 1 \) or \( \alpha > 2 \). The property of the Logistic function has been studied detailedly (Turcotte, 1992, et al.).

Lyapunov exponent is one of the main parameters to study the stability of nonlinear systems. The system is randomized at first:

\[
C_0(i) = \text{rnd} \cdot i = 1,2,\Lambda , N .
\]  

After \( N_f \) iteration, a disturbance \( \{\delta_i, i = 1,2,\Lambda , N\} \) is added onto \( \{C_{N_f}(i), i = 1,2,\Lambda , N\} \), say

\[
C'_{N_f}(i) = C_{N_f}(i) + \delta(i) .
\]

Let \( C_{N_f}(i) \) and \( C'_{N_f}(i) \) evolve simultaneously, and denote

\[
\|d_i\| = \sqrt{\sum_{i=1}^{N_f} [C'_{i}(i) - C_{i}(i)]^2} ,
\]

then

\[
\lambda = \lim_{N_f \to \infty} \frac{1}{N_f} \sum_{i=1}^{N_f} \|d_i\| .
\]

\( \lambda \) is the maximum Lyapunov exponent. The disturbance is “absorbed” if \( \lambda \leq 0 \) by the system while the disturbance is “enlarged” if \( \lambda > 0 \) and large amount of metallogenic material would migrate into or out from the system.

3 Geochemical D-R system

In a geochemical system, \( \epsilon \) and \( \alpha \) can be regarded as parameters represents the characteristics of environment and intensity of metallogeny. For concrete metallogenic system, the reaction function \( F(C) \) concerns all of the involved components and the related reversible and nonreversible reactions. It is a function of various equivalent constants \( (k_i) \), content of components \( (C_j) \), activities coefficients \( (a_j) \), temperature \( (T) \), pressure \( (P) \), pH and Eh values, et al, say
\[
F(C) = F(k_i, C_j, a_j, T, P, pH, Eh \Lambda ).
\]

Formula (10) is an exceedingly summarization of formula (4).

Almost all geothermal processes contain several periods. The existence of relatively quiet periods is the cause of different stages and generations of mineral formation.

In the periods, reaction inner fluid and between fluid and environmental medium reach their equivalences. Nonreversible reactions stop and no more “new” mineral is formed and precipitated. It is to say that the following equation exist

\[
C_{t+1} = 1 - \alpha C_t^2 = C^*.
\]

Its solution is \( C^* = \frac{-1+\sqrt{1+4\alpha}}{2\alpha} \), which is called “fixed point”.

Computer simulation shows that system state at one node during adjacent iterations is tend to oscillate. Fig. 1 shows the states of a variables of 2 adjacent iteration when \( \alpha = 0.9 \) and \( \varepsilon = 0.7 \). According to the theory of stability (see Seydel, 1994), when \( \alpha > 0.75 \), the fixed point \( C^* \) of formula (4) is not stable and bifurcation occurs in the nonlinear system, see Fig. 2. Bifurcation manifests as spatio-temporal fractality in the structure of the system. Fig. 2 shows that bifurcation is not only an integral behavior of the system, but also, with the developing of the system, forced the ore-forming element to be at some certain states in the hydrothermal liquid. If \( C_i(i) \) is greater then \( C^* \) at time \( t \), then \( C_{t+1}(i) \) may less than \( C^* \) at time \( t+1 \). Alternative state oscillation of the variable may causes precipitation of or-forming element, and therefore becomes an important part of the related metallogenic process. When the bifurcation
occurs downwards, the excrement material is forced to solidify; when it occurs upwards, ore-forming material is not enough in the fluid and has to dip out from somewhere. The integral irreversibility of metallogenic system illuminates this kind of dipping is possible, and the higher activity of ions in liquid (than in solid mineral grain) provides an advantageous condition. Hence the amount of mineral precipitated from liquid can be estimated as

\[ M = \sum_{t=1}^{T} (C_t - C_{t+1}), \text{if } C_t \geq C^* \quad \text{and} \quad C_{t+1} < C^* \]  

where \( T \) is the times of bifurcations downwards.

### 4 Law of metallogenic material accumulation

Study of the ore genesis and regularity of ore formation of four metallogenic districts around the Yangtze Craton in China shows that large ore deposits and metallogenic districts are all at the edge of chaos (Yu Chongwen, 1999). These districts include the Cu-Fe metallogenic district of Tongling, Anhui; the Cu-Au-Pb-Zn-Ag metallogenic district of Dexing, Jiangxi; the W-Sn-Mo-Bi-Cu-Pb-Zn etc. metallogenic district of Shizhuyuan, Hunan, and the V-Ti-Fe metallogenic district of Panzhihua, Sichuan, Provinces. If it is true, metallogenic material accumulation of system (1) should reach its highest at the edge of chaos as well.

Numerous studies of dynamical systems show that as the control parameters of an open and spatio-temporal extended non-equilibrium systems increase and exceed a serials of critical thresholds, the system will pass through successive fixed points and limit cycles and eventually approach chaos (Seydel, 1994). Wolfram (1984), Langton (1986), Packard (1988), and Kauffman (1991) discovered almost at the same time the existence of a very narrow region between regions of periodicity and chaos. Since the transition from order to chaos is similar to the phase transition, it follows that this region is just
situated at the transition point (or critical point) between order and chaos. Packard and Kauffman called this transition point “the edge of chaos”. Bak (1991) called it "weak chaos" and considered it to be caused by self-organized criticality.

Computer simulation was done to study the stability of hydrothermal system (1) and the regulation of accumulation of metallogenic material. It is shown that with the change of parameter $\alpha$, the Lyapunov exponent varies regularly. The system is in the state of disorder when $\alpha < 0.75$, and becomes of chaos when $\alpha > 1.5$ approximately. Between these two extremenesses is the state of order and the edge of chaos. The parameter $\varepsilon$ plays an important role to the state of the system. It influences the Lyapunov exponent obviously when $\alpha > 0.75$, see Fig.3. The most important phenomena is that the accumulation of metallogenic material concentrate in the district of order and chaos edge chaos and reach its highest point when the system be at state of chaos edge, see Fig. 4.

This result has been proved by the result of ore-bearing recognition of regional sedimentary geochemical anomalies in the east of China. Two parameters, exponent of spatio-temporal evolution (denoted as $E$) and index of chaos edge (denoted as $P$), were defined. On the plot of which $E$ is the X-axis and $P$ is the Y-axis, the known ore-bearing anomalies cluster within the ranges of $E > 0.0$ and $P > 2.0$, see Fig. 5.

5 Conclusion

Diffusion-reaction system plays an important role in the formation of metamorphic, magmatic and sedimentary ore deposits. It can be simulated by means of “Coupled map lattices” to study the common characteristics of diffusion-reaction systems. Bifurcation, caused by the non-linearity of the system, is not

---

only an integral behavior of the system, but also, with the development of the system, forces the ore-forming element to be at some certain states in the hydrothermal liquid. Alternative state oscillation of the variable may cause precipitation of ore-forming element, and therefore becomes an important part of the related metallogenic process. The concentration of the material will reach its maximum at the edge of chaos, which means that ore bodies, ore deposits and metallogenetic district may be at the edge of chaos.

REFERENCES
