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# Application of the edge of chaos domain of the Zhabotinskii CNN to explore insights to hydrothermal deposit-forming processes

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ABSTRACT

To gain insight into complex processes in hydrothermal deposit-forming systems, we mapped the Zhabotinskii model onto a two-dimensional reaction-diffusion CNN (cellular neural/nonlinear network) of two state variables and two diffusion coefficients. The edge of chaos domain of the Zhabotinskii CNN was numerically determined according to a theory of complexity. The simulation of dynamic systems, with parameters taken from the edge of chaos domain as described in this study, can generate some interesting distribution patterns of component concentrations that plausibly characterize certain complex phenomena involved in hydrothermal mineralization.



## 1. Introduction

Based on observations of rocks, minerals, and the distribution of elements in minerals, one can deduce plausible processes of deposit formation in certain types of mineralization. One often sees periodic oscillations and zonations in mineral deposit samples, and those patterns consist of either different minerals or different contents of minerals. Some oscillations may be due to changes in temperature and pressure changes in mineralization systems, and these types of changes are often directional or symmetrical. For example, cores of mineralized systems often show high-temperature minerals or elements, but gradually toward the edge of such systems more low-temperature mineral or element associations occur. Another example is that veins hosted in fractures of rocks may show low-temperature minerals or elements along their edges close to the country rocks, but high-temperature components inward the veins. There are also other types of periodic oscillations, such as in twins of feldspars that show periodic oscillations without a dominant trend of intensity. These types of localized dissipative formations, which widely exist in various nonlinear dynamic systems, share a common principal characteristic of dynamic arrays, such as cellular nonlinear networks. This common principal character is defined by the presence of interconnections of a sufficiently large number of simple dynamic units, which can be explained using a cellular neural/nonlinear network (CNN) dynamic simulation. CNN involves spatial arrangement of locally coupled cells, where each cell is a dynamical system that has input, output, and state variables according to certain prescribed dynamical laws (Chua, 1997). Dynamical systems of interconnection of several simple dynamic units often exhibit extremely complex, synergistic, and self-organizing behaviors. Reaction-diffusion CNNs have been used to simulate phenomena about complexity in nonlinear chemistry, physics, and other fields (Chua, 1997; Dogaru and Chua, 1998a, b, c; Min et al., 2000). Another common characteristic of dissipative formations, which involve active wave propagation phenomena, is the presence of an active medium that is powered by a constant supply of external energy. In a hydrothermal deposit-forming system, for example, the local components act as active media (far from the thermal dynamic equilibrium regions), which is powered by the entrance of hydrothermal fluids.

Some progress has been made to understand the emergence and complexity of hydrothermal deposit-forming processes (Yu, 1999a, b, c, 2000a, b; Xu et al., 2003, 2010). In this paper, we described a method to determine the edge of chaos domain in order to simulate some significant phenomena involved in hydrothermal deposit-forming systems by using the reaction-diffusion Zhabotinskii CNN. In this method, we transformed a reaction-diffusion CNN from partial differential equations (PDEs) by discretizing the spatial coordinates of the state variables.

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## 2. Conceptual PDE and CNN for hydrothermal deposit-forming processes

In hydrothermal deposit-forming systems, reaction and diffusion processes play important roles that can be modeled using PDEs:

$$\frac{\partial C_i}{\partial t} = f_i(C_1,C_2,\ldots,C_n) + D_i\left(\frac{\partial^2 C_i}{\partial x^2} + \frac{\partial^2 C_i}{\partial y^2} + \frac{\partial^2 C_i}{\partial z^2}\right), \quad i = 1,2,\ldots,n. \tag{1}$$

here $(x,y,z) \in \Omega \subseteq \mathbf{R}^3$, and $\mathbf{C} = (C_1,C_2,\ldots,C_n)^\tau$ is the vector of concentrations of a system's chemical components that are treated as state variables of the system. The nonlinear functions $\mathbf{f}(\mathbf{C}) = (f_1(\mathbf{C}), f_2(\mathbf{C}),\ldots,f_n(\mathbf{C}))^\tau$ represent either the kinetic term or the reaction term of a dynamic system. The second term on the right side of Eq. (1) represents the diffusion term with $D_1,D_2,\ldots,D_n$ as diffusion coefficients. $\mathbf{D} = diag(D_1,D_2,\ldots,D_n)$ is a diagonal matrix composed of diffusion coefficients. Under given pressure and at an appropriate temperature, the kinetic term is mainly associated with the rates of chemical reactions and the diffusion term is mainly determined by the porosity and penetrability of the system media.

According to Dogaru and Chua (1998a), we can formulize a CNN using a regular grid coordinate system that partitions a deposit-forming region $\Omega$ into $N_k \times N_l \times N_m$ regular units with a constant spatial interval. According to the new coordinate system, we can represent Eq. (1) in a discrete form in which the Laplacian term has been replaced by its central differences along the $x$, $y$, and $z$ directions, respectively. This result gives a group of $n \times N_k \times N_l \times N_m$ first-order ordinary differential equations that form the reaction-diffusion CNN.

$$\dot{C}_i(k,l,m) = f_i(C_1(k,l,m), C_2(k,l,m),\ldots, C_n(k,l,m)) + I_i, \quad i = 1,2,\cdots,n, \tag{2}$$

where

$$\begin{aligned} I_i = {} & D_i[C_i(k-1,l,m) + C_i(k+1,l,m) + C_i(k,l-1,m) + C_i(k,l+1,m) \\ & + C_i(k,l,m-1) + C_i(k,l,m+1) - 6C_i(k,l,m)], \\ & k = 1,2,\ldots,N_k; \quad l = 1,2,\ldots,N_l; \quad m = 1,2,\ldots,N_m. \end{aligned} \tag{3}$$

The above CNN is three-dimensional. Similarly, we can obtain a two-dimensional reaction-diffusion CNN. However, the process of a real deposit-forming system is very intricate. Nevertheless, hydrothermal mineral deposits are thought to form mainly in self-catalyzed redox reactions. For convenience without loss of generality, a two-component model proposed by Zhabotinskii (1974) is applied here to simulate some phenomena in hydrothermal deposit-forming processes. The following Zhabotinskii model (in the unstirred special case) is reduced from the three-component Oregonator model (Field and Burger, 1985).

$$\begin{aligned} \frac{\partial C_1}{\partial t} &= f_1(C_1,C_2) + D_1\Delta C_1 \\ \frac{\partial C_2}{\partial t} &= f_2(C_1,C_2) + D_2\Delta C_2, \end{aligned} \tag{4}$$

where

$$\begin{aligned} f_1(C_1,C_2) &= C_1\{1 - C_2[2 + (C_1-1)^2]\} + a, \\ f_2(C_1,C_2) &= -bC_2 - C_1(C_2-1). \end{aligned} \tag{5}$$

This model involves two chemical components ($C_1$ and $C_2$), two system parameters ($a$ and $b$), and two diffusion coefficients ($D_1$ and $D_2$). This model can represent the simple conditions involved in hydrothermal deposit-forming or mineralization systems. The system parameters $a$ and $b$ may be used to represent with temperature, pressure, and other factors, like velocity of reaction, which are dimensionless integrative variables. $D_1$ and $D_2$ are diffusion coefficients of the two chemical components. The reaction terms $f_1$ and $f_2$ involve a third-order nonlinear relationship between the components $C_1$ and $C_2$, implying that a change in the concentration of one component is related to a change in the concentration of the other component. An example of this would be a hydrothermal zinc deposit-forming system containing two main chemical components of Ca and Zn in a hydrothermal solution. As the mineral sphalerite (ZnS) crystallizes, the remaining solution will have reduced concentrations of Zn and increased concentrations of Ca. When the concentration of the latter reaches a critical level, calcite ($CaCO_3$) starts to form and causes the system to change toward the Zn-rich direction. The complex relationship of the two components described or modeled in Eq. (5) is explained in Field and Burger (1985).

To determine the variation region of $a$ and $b$ in Eq. (5) so that a hydrothermal deposit-forming system may exhibit complexity is one of the two main tasks of the research. The other task is to simulate some significant phenomena in hydrothermal deposit-forming processes by the following CNN. Discretization of the model gives the following form

$$\begin{aligned} \frac{dC_1(i,j)}{dt} &= f_1(C_1(i,j),C_2(i,j)) + I_1 \\ \frac{dC_2(i,j)}{dt} &= f_2(C_1(i,j),C_2(i,j)) + I_2, \end{aligned} \tag{6}$$

where

$$I_k = D_k(C_k(i-1,j) + C_k(i+1,j) + C_k(i,j-1) + C_k(i,j+1) - 4C_k(i,j)). \tag{7}$$

Eqs. (5)–(7) together form the CNN that is applied in this study as described in the following sections. Because this CNN is formed from the PDEs suggested by Zhabotinskii (1974) to describe the Belousov–Zhabotinskii reaction, we refer to it as the Zhabotinskii CNN.

## 3. Determining the edge of chaos domain of the Zhabotinskii CNN

As Dogaru and Chua (1998a) pointed out, whether a homogeneous medium is capable or incapable of exhibiting complexity depends on whether the CNN cell, or its couplings, is locally active in a precise mathematical sense. However, it is usually difficult to select suitable system parameters in the phase space so that a system acts as we expect it to for the emergence of dissipative formation. The best way to select suitable parameters is to find the edge of chaos and the local active domains of the CNN cells, from which suitable system parameters can be chosen roughly to enable the system to exhibit complexity. The following three steps are needed to determine the edge of chaos domain.

(1) Determine the equilibrium domain. To calculate the equilibrium points of Eq. (6) in the case of no diffusion, $I_1 = I_2 = 0$, for simplicity but without loss of generality, the spatial coefficients $(i,j)$ are dropped from the notation in the following equations.

$$\begin{aligned} \dot{C}_1 &= f_1(C_1,C_2) \\ \dot{C}_2 &= f_2(C_1,C_2). \end{aligned} \tag{8}$$

If we assume that the system is at equilibrium (so that $f_1(C_1,C_2) = 0$, $f_2(C_1,C_2) = 0$), we get

$$\begin{aligned} & C_1\{1 - C_2[2 + (C_1-1)^2]\} + a = 0, \\ & -bC_2 - C_1(C_2-1) = 0. \end{aligned} \tag{9}$$

Through calculation using Matlab software, two equilibrium points of the Zhabotinskii CNN cells for each pair of $a$ and $b$ can be found. These points are functions of $a$ and $b$, which are denoted by $(C_1(Q_1), C_2(Q_1))$ and $(C_1(Q_2), C_2(Q_2))$ in the