

An Analog CMOS Circuit emulating the Belousov-Zhabotinsky Reaction

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Abstract—*The Belousov-Zhabotinsky (BZ) reaction gives us important clues to reveal the functions of nonlinear vital phenomena in nature. Because of the difficulty in computing such reaction-diffusion systems using conventional digital processors, we here propose an analog CMOS circuit that emulates the BZ reaction. A 2-D array of the analog (BZ) circuit is responsible for fast emulation, and its operation rate is independent of the system size. The operations of the proposed circuit were demonstrated by the fabricated chip and SPICE.*

I. INTRODUCTION

The formation of spatial and temporal patterns in dissipative and autocatalytic reaction systems have been spotlighted since almost every natural phenomenon, from traditional convective phenomena to modern neuro dynamics, can be categorized into these systems. Although a number of theoretical and numerical studies have been conducted to reveal the mechanism of those systems, the essential behaviors are still unknown due to their complexity and requirement of massive computational power in the numerical simulations. In this report, aiming at the development of high-speed emulators that advance understanding of such systems, we propose an analog CMOS circuit that implements a reaction-diffusion (RD) system [1].

Implementing RD systems in hardware (VLSI) has several merits. First, hardware RD system is very useful for simulating RD phenomena, even if the phenomena never occurs in nature. This implies that the hardware system is one possible candidate for developing an artificial RD system that is superior to natural system. Second, hardware RD system can operate much faster than actual RD systems. For instance, the velocity of chemical waves in Belousov-Zhabotinsky (BZ) reaction is $O(10^{-2})$ m/s [2], while that of hardware RD system will be over a million times faster than that of the BZ reaction, independently of system

size [3], [4], [5]. This property is useful for developers of RD applications because every RD application benefits from the operation speed.

II. THE REACTION-DIFFUSION SYSTEM

A reaction diffusion (RD) system is described by a set of partial differential equations

$$\frac{\partial x_i(\mathbf{r}, t)}{\partial t} = D_i \nabla^2 x_i(\mathbf{r}, t) + f_i(x_i(\mathbf{r}, t)), \quad (1)$$

where \mathbf{r} represents the space, t the time, ∇^2 the spatial Laplacian, D_i the diffusion constant, f_i the nonlinear reactive functions that depend on several different reactive species x_i . One well-known reactive function is described in a two-variable Oregonator, which is derived from the BZ reaction [1], [6]. The point dynamics are given by

$$\frac{dx_1}{dt} = \frac{1}{\tau} \left(x_1 (1 - x_1) - a x_2 \frac{x_1 - b}{b + x_1} \right), \quad (2)$$

$$\frac{dx_2}{dt} = x_1 - x_2, \quad (3)$$

where x_1 and x_2 represent the concentration of HBrO_2 and Br^- ions, respectively, while τ , a and b represent the reaction parameters. The value of τ is generally set at $\tau \ll 1$ since the reaction rate of HBrO_2 ion is much faster than that of Br^- ions. The nullclines of the Oregonator where $dx_1/dt = 0$ and $dx_2/dt = 0$ are given by

$$x_2 = \frac{x_1 (x_1 + b)(1 - x_1)}{a (x_1 - b)}, \quad (\equiv l_1) \quad (4)$$

$$x_2 = x_1. \quad (\equiv l_2) \quad (5)$$

A cross point of those two nullclines (l_1 and l_2) represents a fixed point of the Oregonator.

Figure 1 shows the nullclines and trajectories of the Oregonator with typical parameter-values ($\tau = 10^{-2}$ and $b = 0.02$). The value of parameter a was set at 1 [Fig. 1(a)] and 3 [Fig. 1(b)]. Depending on the position of the fixed point, the Oregonator exhibits oscillatory or excitatory behavior. When $a = 1$, the fixed

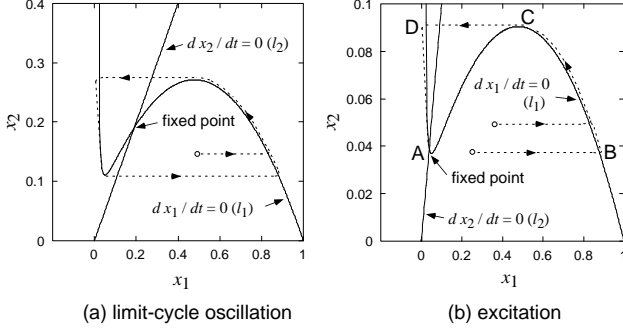


Fig. 1. Nullclines and trajectories of the Oregonator in (a) oscillatory mode and (b) excitatory mode.

point is located on nullcline l_1 at which $dx_2/dx_1 > 0$. In this case, the Oregonator exhibits limit-cycle oscillations [Fig. 1(a)]. The oscillation represents periodic oxidation-reduction phenomena of the BZ reaction. On the other hand, the fixed point is located on nullcline l_1 at which $dx_2/dx_1 < 0$ when $a = 3$. Under this condition, the Oregonator exhibits excitatory behavior [Fig. 1(b)] and is stable at the fixed point as long as external stimulus is not given.

In the Oregonator, three circulative states are introduced according to the phase of oscillation; i.e., inactive (A), active ($B \rightarrow C$), and refractory periods ($D \rightarrow A$), as labelled in Fig. 1(b). The inactive, active, and refractory states represent a depletion in the Br^- ion, an autocatalytic increase in the HBrO_2 ion (oxidation of the catalyzer), and a depletion in the Br^- ion (reduction of the catalyzer), respectively. When the Oregonator is inactive, it easily become active ($A \rightarrow B$) by external stimuli. Then, it turns in refractory state ($C \rightarrow D$). During the refractory state, the Oregonator can not be activated even if the external stimuli was given.

III. ANALOG CMOS CIRCUITS FOR THE BZ REACTION

We here propose a novel analog cell that is qualitatively equivalent to the Oregonator. We define the dynamics of a cell as

$$\frac{dx_1}{dt} = \frac{1}{\tau} \left(-x_1 + f(x_1 - x_2, \beta_1) \right), \quad (6)$$

$$\frac{dx_2}{dt} = -x_2 + f(x_1 - \theta, \beta_2), \quad (7)$$

where $f(\cdot)$ represents a sigmoid function defined by

$$f(x, \beta) = \frac{1 + \tanh \beta x}{2}. \quad (8)$$

The cell dynamics are designed so that the shape of nullclines and flows (\dot{x}_1, \dot{x}_2) are qualitatively equivalent

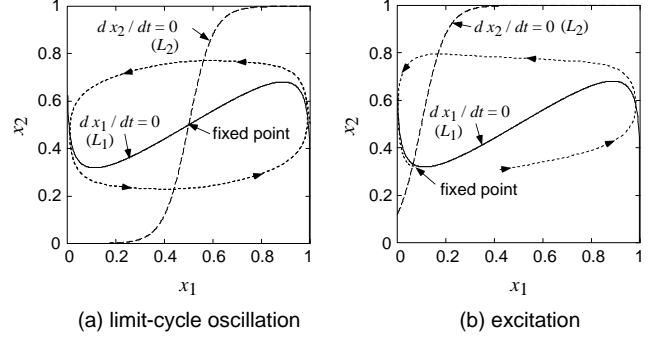


Fig. 2. Nullclines and trajectories of the proposed analog cell in (a) oscillatory mode and (b) excitatory mode.

to that of the Oregonator. The cubic nullcline (l_1 in Fig. 1) is approximated by a nullcline of Eq. (6) as

$$x_2 = x_1 - \beta_1^{-1} \tanh^{-1}(2x_1 - 1), \quad (\equiv L_1) \quad (9)$$

while the linear nullcline (l_2 in Fig. 1) is approximated by a nullcline of Eq. (7) as

$$x_2 = f(x_1 - \theta, \beta_2). \quad (\equiv L_2) \quad (10)$$

An analog cell, whose dynamics are described by Eqs. (6) and (7), is very suitable for analog VLSI implementation because the sigmoid function can easily be implemented on the VLSIs by using differential-pair circuits.

The proposed cell exhibits qualitatively equivalent behaviors to the Oregonator, as shown in Fig. 2. The values of parameters are $\tau^{-1} = 10$, $\beta_1 = 5$ and $\beta_2 = 10$. When $\theta = 0.5$, the fixed point exists on a nullcline [Eq. (9)] where $dx_2/dx_1 > 0$, and the system exhibits limit-cycle oscillations [Fig. 2(a)]. On the other hand, the system exhibits excitatory behavior [Fig. 2(b)] when the fixed point exists on a nullcline (10) where $dx_2/dx_1 < 0$ [Fig. 2(b)].

Now, let us introduce the cell dynamics into the RD model aiming at the constructing 2-D RD system. The dynamics of the RD system are described by substituting the reactive term in Eq. (1) with the right terms of Eqs. (6) and (7). The discrete expression of the RD system is given by

$$\frac{du_{i,j}}{dt} = \frac{1}{\tau} \left(-u_{i,j} + f(u_{i,j} - v_{i,j}, \beta_1) \right) + g_{i,j}^u, \quad (11)$$

$$\frac{dv_{i,j}}{dt} = -v_{i,j} + f(u_{i,j} - \theta, \beta_2) + g_{i,j}^v, \quad (12)$$

where the system variable x_i is replaced by $u_{i,j}$ and $v_{i,j}$, while $g_{i,j}^u$ and $g_{i,j}^v$ represent external inputs to the cell (interactions between a cell and its neighboring

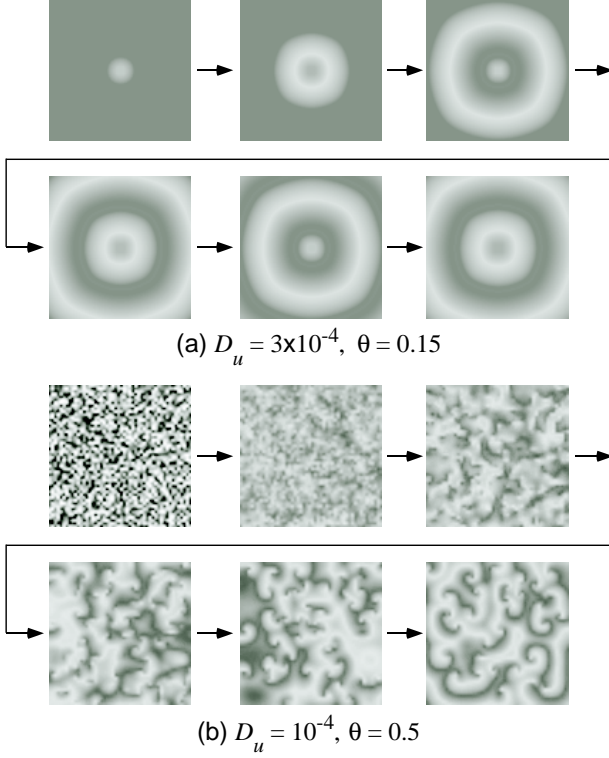


Fig. 3. Numerical results of a RD system using the analog cell in (a) excitatory mode and (b) oscillatory mode.

cells) as

$$g_{i,j}^u = D_u \frac{u_{i-1,j} + u_{i+1,j} + u_{i,j-1} + u_{i,j+1} - 4u_{i,j}}{h^2},$$

$$g_{i,j}^v = D_v \frac{v_{i-1,j} + v_{i+1,j} + v_{i,j-1} + v_{i,j+1} - 4v_{i,j}}{h^2}.$$

Figure 3 shows spatiotemporal activities of the 2-D RD system with 50×50 cells ($\beta_1 = 5$, $\beta_2 = 10$, $h = 0.01$ and $D_v = 0$) where the values of $v_{i,j}$ are represented in grayscale ($v_{i,j} = 0$: black, $v_{i,j} = 1$: white). The Neumann boundary condition was applied at the side of the square reaction-space. When $\tau^{-1} = 10^2$ and $\theta = 0.15$ at which the cell exhibits excitatory behavior, the 2D system produced target patterns [Fig. 3(a)], as observed in the basic RD system with the Oregonators. In the simulation, diffusion coefficient D_u was set at 3×10^{-4} . The results indicate that the proposed RD system is qualitatively equivalent to the basic RD system with the Oregonators since the excitatory property of the analog cells is inherently the same as that of the Oregonator.

Figure 3(b) shows dynamic behaviors of the 2-D RD system with $D_u = 10^{-4}$ and $\theta = 0.5$ at which the cell exhibits oscillatory behavior. Initial values of the cells were randomly chosen as $u_{i,j} = \text{RAND}[0, 1]$ and $v_{i,j} = \text{RAND}[0, 1]$. The system produced 2-D phase-lagged stable synchronous patterns called *mod-*

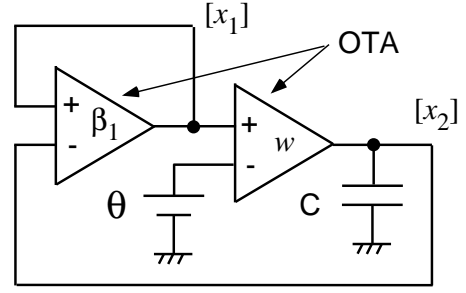


Fig. 4. An analog cell circuit consisting of single capacitor and two operational-transconductance amplifiers (OTAs).

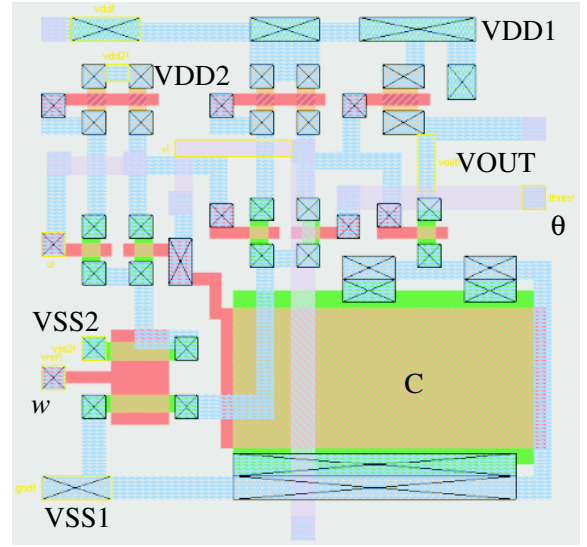


Fig. 5. Layout of the analog cell designed with 1.5- μm CMOS process (cell size: $70 \times 70 \mu\text{m}^2$).

elock, due to the weak coupling between the neighboring cells. When $D_u > 10^{-3}$, all cells exhibit synchronous oscillation, namely, no spatial pattern was produced.

An analog circuit of the proposed cell and its device layout are shown in Figs. 4 and 5, respectively. The circuit consists of single capacitor and two operational-transconductance amplifiers (OTAs), which implies that the circuit can easily be implemented on silicon VLSIs using conventional CMOS technology. The circuit can be obtained by qualitative approximation of Eqs. (6) and (7).

When the rate constant of Eq. (6) is much larger than that of Eq. (7), the differential term of Eq. (6) can be neglected ($\tau \ll 1$), as introduced in Sec. II. On the other hand, Eq. (7) with $\beta_2 \rightarrow \infty$ forces the values of variable x_2 to be 0 when $x_1 \leq \theta$, while $x_2 \rightarrow 1$ when $x_1 > \theta$. If the variable x_2 is forced to have the value within $[0:1]$, the temporal difference in Eq. (7) can approximately be represented by binary values.

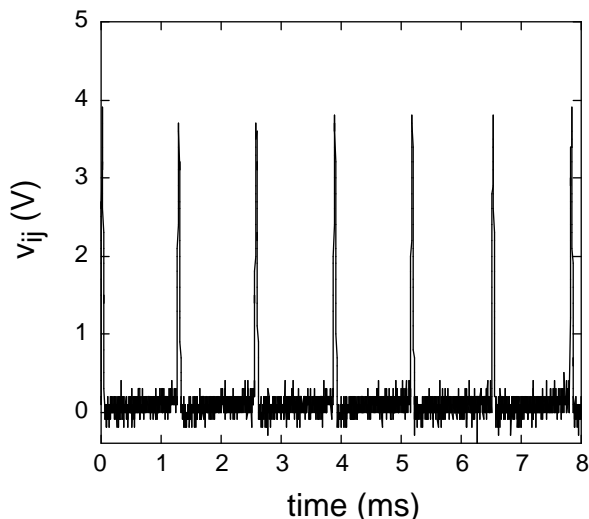


Fig. 6. Experimental results of the BZ cell

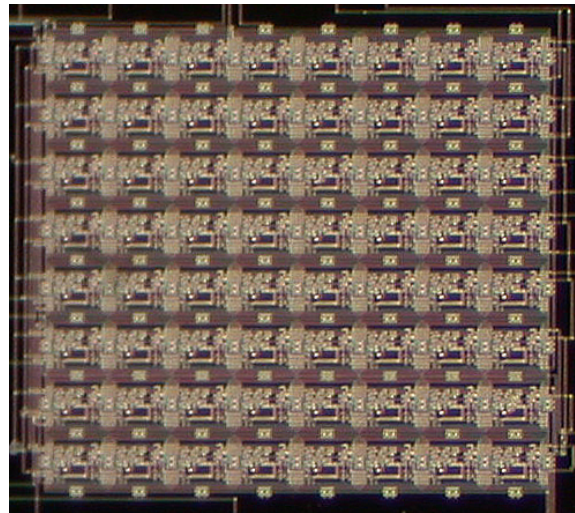


Fig. 7. Chip photograph of 2-D BZ circuits.

Consequently, we obtain a new dynamical equation from Eqs. (6) and (7) as

$$x_1 = f(x_1 - x_2, \beta_1) \quad (13)$$

$$\frac{dx_2}{dt} = \begin{cases} w & (\text{if } x_1 > \theta) \\ -w & (\text{else}) \end{cases} \quad (14)$$

where w represent positive and small constant. In Fig. 4, an OTA labeled as β_1 serves as the function of Eq. (13), while a capacitor C and the rest OTA receiving voltage θ produce the dynamics for Eq. (14). The positive constant w is implemented in the OTA (labeled as w) where w corresponds to the source current of a differential pair. The output current of the OTA (w) becomes zero when the voltage of output node x_2 is equal to the supply voltage (VDD or VSS). The value of x_2 is thus restricted within [VDD:VSS].

Figure 6 shows experimental results of the fabricated chip that implements the reaction circuit shown in Fig. 5 (MOSIS 1.5- μm CMOS, cell size: $70 \times 70 \mu\text{m}^2$). Supply voltages of an OTA of β_1 was set at VDD = 4 V and VSS = 0.5 V, while that of the rest OTA (w) was set at VDD = 5 V and VSS = GND. The threshold θ was set at 2.5 V so that the circuit exhibits oscillatory behaviors. In the device layout shown in Fig. 5, the capacitor C was implemented by a MOS capacitor (lower-right rectangle in Fig. 5). As expected, the circuit exhibited qualitatively same behaviors as the Oregonator; i.e., stiff nonlinear oscillations.

IV. SUMMARY

We proposed an analog CMOS circuit that imitates a model of Belousov-Zhabotinsky (BZ) reaction. Numerical simulations and experimental results

of the fabricated chip showed that the circuit can successfully produce excitatory responses and thus spiral waves in the same way as natural reaction-diffusion (RD) systems. These results encourage us to develop novel applications based on natural RD phenomena using the hardware RD devices.

The proposed devices and circuits are useful not only for the hardware RD system but also for constructing modern neuro-chips. The excitatory and oscillatory behaviors of the RD circuit are very similar to actual neurons that produce sequences in time of identically shaped pulses, called *spikes*. Recently, Fukai showed that an inhibitory network of spiking neurons achieves robust and efficient neural competition on the basis of a novel timing mechanism of neural activity [7]. A network with such a timing mechanism may provide an appropriate platform for the development of analog VLSI circuits that overcome the problems of analog devices, namely their lack of precision and reproducibility.

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