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Crossover Structures for Logical Computations in Excitable Chemical Medium

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It is known that spatially distributed excitable chemical medium is capable of performing chemical computation. As a kind of unconventional computation, chemical computation should have the ability to replicate basic functions in conventional computation, such as logic circuits. Owing to the planar structure of the excitable medium, it is difficult to implement crossing wires in excitable medium, which is very common in digital electronics. The chemical implementation of the crossover attracts more and more attention in these years. This paper concentrates on the design and realization of crossover in excitable medium, and discusses its applications in logical computations. Three kinds of combinational logic circuits, including binary adder, binary encoder and binary decoder are constructed. The simulation results demonstrate the effectiveness of crossover structures, as well as all the combinational logical devices.

Keywords: Belousov-Zhabotinsky reaction, chemical computation, excitable media, crossover structure, logic circuits, binary adder, binary encoder, binary decoder

1 INTRODUCTION

It has been proposed that the Belousov-Zhabotinsky (BZ) excitable medium can implement various computational operations [1–3]. Unlike conventional computing in electronic computers, this kind of computation, which is so-called chemical computation, relies on geometrically constrained excitable chemical medium, and represents data in sequences of concentration pulses of the BZ reagents [4, 5]. As an unconventional strategy of information processing, chemical computation is capable of replicating components used in conventional computation, such as logic circuits.

Since the Showalter Laboratory realized the first logic gates in excitable medium in 1994 [6, 7], the chemical implementations of logic circuits have attracted the attention of many researchers. These logical devices are based on the space-time interaction of travelling excitation waves. By a clever geometrical arrangement of the channels for the excitation wave propagation, researchers have built several logical devices, such as chemical diode [8–10], Boolean logic gates [11–14], adders [15–17], counters [18], memory cells [12], etc. Many of them have already been verified in simulations or in chemical experiments.

However, the BZ excitable medium is planar structure. No signal channels could intersect. It is difficult to design complex logical devices without crossover structure; or the devices may occupy large space, even though they can be constructed. Some researchers have realized the problem and done some research on crossing pulses. Reference [19] discussed the properties of a cross junction, the cross junction could act as a coincidence detector and a switch according to the properties. Reference [17] proposed two structures for cross propagation, but these structures cannot work when two input pulses propagate nearly simultaneously. Reference [20] introduced two structures for crossing over too. These structures are simple and powerful, but we need to create periodic inhibiting valves for time-dependent wave selection, which limits their applications.

In this paper, we focus on the design and applications of the crossover structures based on the BZ reaction. Two kinds of structures are proposed. The simple one permits only one output pulses at one time, while the other permits two input pulses to propagate highly or nearly simultaneously and keeps two output pulses synchronized. Furthermore, the crossover structures are applied to logical computations. Three kinds of combinational logic circuits, including binary adder, binary encoder and binary decoder are constructed and verified in simulation. It is easy to implement higher-bit combinational logic circuits by cascading lower-bit circuits, since crossover structures are introduced.

The rest of the paper is organized as follows. In section 2, we present the details of the two-variable Rovinsky-Zhabotinsky (RZ) model used in simulation of the BZ reaction. The design and the function of crossover structures are described in section 3. We build multi-bit binary adder, binary encoder and binary decoder based on the crossover structures in section 4. The paper is concluded in section. 5.

2 THE RZ MODEL OF THE BZ REACTION

The RZ model of the BZ reaction is applied to calculate the propagation of the pulses in this paper. The RZ model, which is derived from the Field-Koros-Noyes (FKN) reaction mechanism [21], has two variables, x and z, corresponding to dimensionless concentrations of activator $HBrO_2$ and of catalyst $Fe(phen)_3^{3+}$. In the active regions, which contain the catalyst, the time evolution of the concentrations of x and z is described by Equation (1).

$$\begin{aligned}\frac{\partial x}{\partial \tau} &= \frac{1}{\varepsilon}\left[x(1-x) - (2q\alpha\frac{z}{1-z} + \beta)\frac{x-\mu}{x+\mu}\right] + \nabla^2 x,\\ \frac{\partial z}{\partial \tau} &= x - \alpha\frac{z}{1-z}.\end{aligned} \tag{1}$$

In the passive regions, where catalyst is absent, the concentrations of x and z evolve according to Equation (2).

$$\begin{aligned}\frac{\partial x}{\partial \tau} &= -\frac{1}{\varepsilon}\left[x^2 + \beta\frac{x-\mu}{x+\mu}\right] + \nabla^2 x,\\ z &= 0.\end{aligned} \tag{2}$$

In numerical calculations, Equations (1) and (2) are solved numerically using Euler method with a five-node Laplace operator for the diffusion term. The time step $\Delta\tau$ is 0.0001, and the distance between each grid point $\Delta\rho$ is 0.3301 [17, 22]. The other parameters are the same values as considered in refs. [17, 18, 22]: $\epsilon = 0.1176$, $q = 0.5$, $\alpha = 0.068$, $\beta = 0.0034$, and $\mu = 0.00051$. For these values of parameters, the stationary concentrations of x and z in the active region (stationary solution of Equation (1)) are: $x = 7.27 \times 10^{-4}$, $z = 1.06 \times 10^{-2}$; and the stationary concentrations in the passive region (stationary solution of Equation (2)) are: $x = 5.12 \times 10^{-4}$, $z = 0$.

Many kinds of computational devices can be implemented by the model, based on the geometrical configuration of the channels. In this paper, we set the width of the channels to 20 grid points to keep the structures compact. In simulations, the pulses in the active regions are initiated by increasing the value of x to 0.1 at the end of signal channels, and then the excitation waves will propagate inside the channels. In simulation results, the black color shows the distribution of the active regions, and the white parts are passive. A high concentration of activator x is marked as a gray wave in the active regions.

3 CROSSOVER STRUCTURES IN EXCITABLE MEDIUM

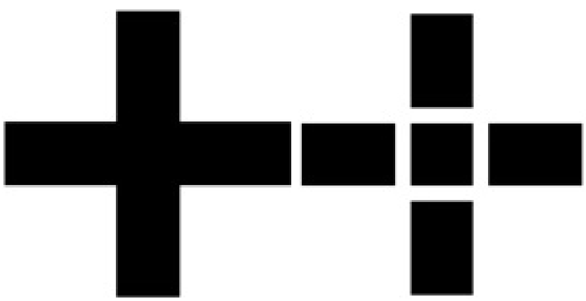
3.1 Simple crossover structure

The properties of excitable medium offer a number of functions that are useful for information processing [5]. In this section, the property of excitable medium, angle dependent penetration of passive region is used to implement cross propagation of the pulses.

Penetration means a pulse propagating in the active region can penetrate into a passive part and disappears after some distance. The pulse can excite the active region behind the passive stripe, if the stripe is narrow enough. It is said that the maximum width of the passive stripe depends on the angle between the wave vector of the pulse and the normal to the stripe. A pulse with the wave vector perpendicular to the stripe can pass a wider stripe than a pulse propagates along the strip. Thus, in a junction of two channels (Figure 1 (a)), the interactions of the channels can be excluded by adding passive stripes with proper width, as shown in Figure 1(b).

Under the simulation condition, we cannot find a proper width of the stripe when channel is 20 grid points wide; while for 40-grid point wide channel, 10-grid point is a good choice. Figure 2 illustrates the simple crossover structure, in which the unit is 10 grid points wide and high. A junction of two 40-grid point wide channels are separated by four 10-grid point wide penetration units, and connected to 20-grid point wide channels. This device permits the pulse to propagate through channel AA' or BB' without outputs in channel BB' or AA'. Images extracted from time-series simulations are shown in Figure 3, videos of the simulations can be found in reference [23].

For unidirectional propagation, we reduce the length of 40-grid point wide channels to 10 grid points, as shown in Figure 4. The pulse from O_1 or O_2 cannot pass the penetration unit as it cannot penetrate so long in an almost



(a) (b)

FIGURE 1
A junction linking two channels. (a) The simple junction. (b) The junction in which the interactions of the two channels are excluded.

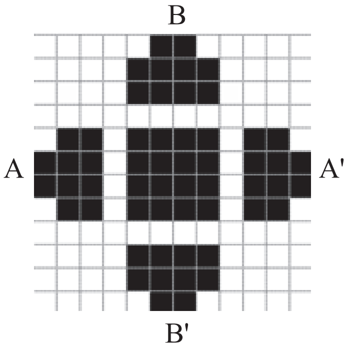


FIGURE 2
A simple structure for crossing over. The unit is 10 grid points wide and high.

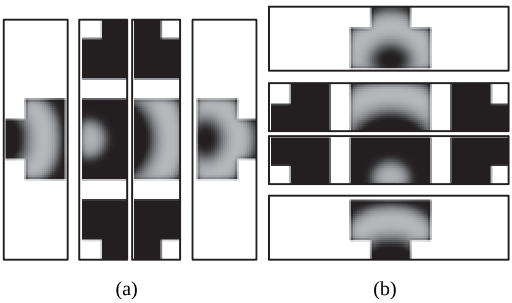


FIGURE 3
Simulation results of the simple crossover. (a) Pulse propagates from A to A'. (b) Pulse propagates from B' to B.

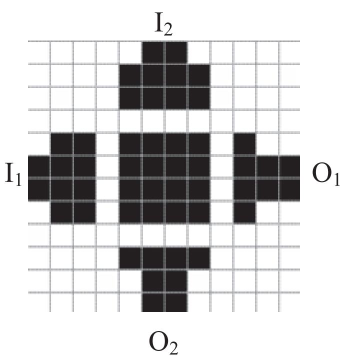


FIGURE 4
A unidirectional crossover structure. The pulse can only propagate from I_1 to O_1 or from I_2 to O_2. The unit is 10 grid points wide and high.

20-grid point wide channel. Reference [23] shows the simulation results of this structure.

This structure achieves the same function of crossover as reference [17], but occupies less space. It is employed to construct binary adder and binary encoder in section 4. However, the device cannot send two pulses when both input channels are excited. If two pulses occur simultaneously, they will affect each other and annihilate; if two pulses propagate nearly simultaneously, the former will spread out, while the latter will annihilate according to the refractory period of the excitable medium [5]. This problem will be solved in the next section.

3.2 Multi-functional crossover structure

A crossover should deal with the case when two pulses propagate highly or nearly simultaneously; meanwhile, whether there is a single input pulse or two input pulses, the propagation time of the pulses should be the same in the crossover structure, so that the time-sequence of the pulses does not change after crossing. To achieve the functions above, we build another crossover structure by using such elements as chemical diode [8], T-shaped coincidence detector [18] and angle dependent penetration unit. Figure 5 illustrates the structure, which consists of two chemical diodes (D_1 and D_2), a modified T-shape coincidence detector (T) and two penetration units (P_1 and P_2). The response of such a device is described as follows. Images extracted from time-series simulation results are shown in Figure 6, videos of the simulations can be found in reference [23].

1. A single pulse: If a pulse comes from input I_1 and propagates along channel C, it will pass penetration unit P_2, and spread out from output O_1. There is no signal at output O_2 as the pulse will die at penetration

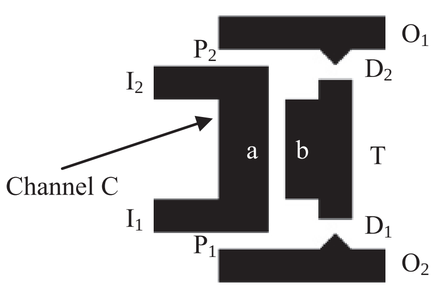
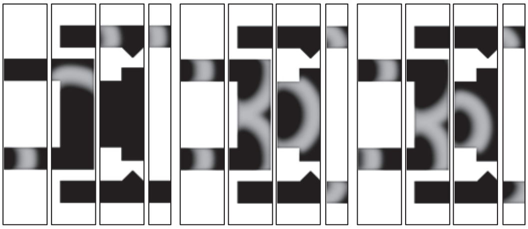


FIGURE 5
A multi-functional crossover structure. This structure consists of two chemical diodes (D_1 and D_2), a modified T-shape coincidence detector (T) and two penetration units (P_1 and P_2).



(a) (b) (c)

FIGURE 6
Simulation results of the crossover. (a) A single pulse from input I_1. (b) Two pulses from input I_1 and I_2 at the same time. (c) The pulse from input I_1 is 15 grid points later then the pulse from input I_2.

unit P_1 (Figure 6 (a)). The same process will be followed for a single pulse from input I_2.

2. Two pulses at the same time: If two pulses appear simultaneously at input I_1 and I_2, they will meet at point *a* and annihilate subsequently, then a new excitation pulse will be generated at point *b*, and finally, two output pulses will be sent through diode D_1 and D_2 simultaneously (Figure 6 (b)).
3. Two pulses one after the other: If two input pulses propagate nearly simultaneously (less than 30 grid points), there will be two output pulses and the pulses will spread out in order. For example, in Figure 6 (c), the pulse from input I_1 is 15 grid points later than the pulse from input I_2. The two pulses meet (and subsequently annihilate), then the detector bar T becomes excited and sends two individual pulses into output O_1 and O_2. The pulse at output O_1 is also nearly 15 grid points later than the pulse at output O_2.

The simulation results illustrate that the pulse propagation time in the crossover structure is the same for all three cases.

The multi-functional crossover structure is more complex than the simple one, but it allows one or both pulses as inputs, and keeps outputs synchronized. This device is used to implement crossing wires in binary decoder in Section 4.

4 COMBINATIONAL LOGIC CIRCUITS BASED ON CROSSOVER STRUCTURES

4.1 Logic gates

In digital electronics, combinational logic circuits are constructed by combining logic gates. Similarly, we design combinational logic circuits by the same

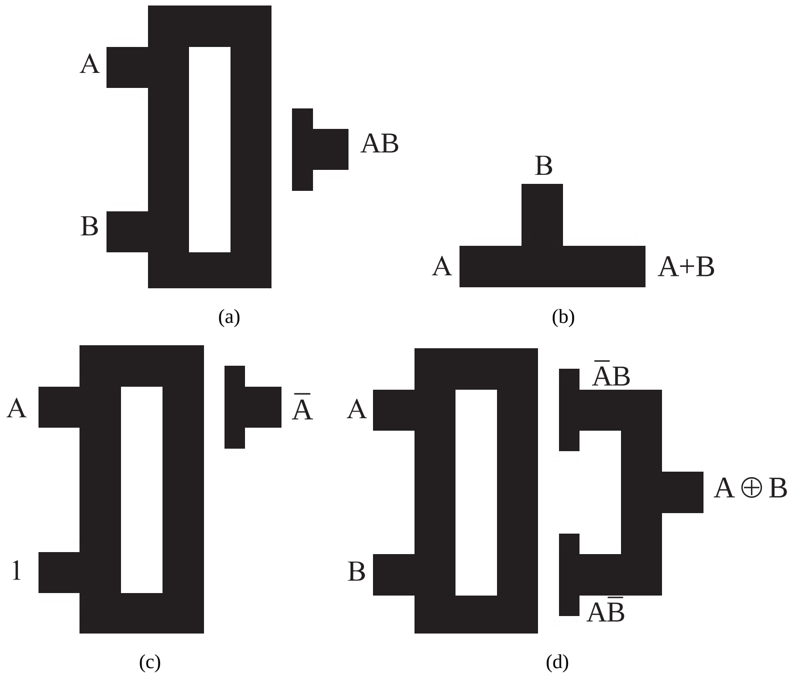


FIGURE 7
Logic gates. (a) AND gate. (b) OR gate. (c) NOT gate. (d) XOR gate.

method in excitable medium. The logic gates used in this paper are described as follows.

1. AND gate: T-shaped coincidence detector is regarded as chemical realization of AND gate, as shown in Figure 7 (a), (c) and (d).
2. OR gate: OR gate is realized by linking channels directly (Figure 7 (b)).
3. NOT gate: As shown in Figure 7 (c), NOT gate is replaced by AND-NOT gate with a constant auxiliary 1 input.
4. XOR gate: Figure 7 (d) shows the structure of XOR gate, which combines AND, OR and NOT gates.

Note that the pulse from one input will propagate into the other in the structures in Figure 7, but it has no influence on the outputs. Therefore, we do not add additional penetration units or diodes in the input channels for simplicity, if the outputs do not interfere with the inputs.

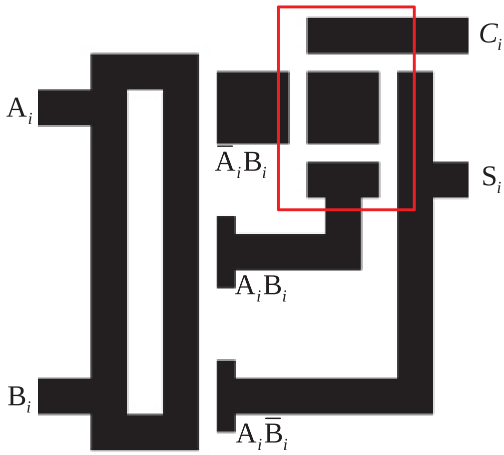


FIGURE 8
The structure of half-adder. A simple crossover structure is used to exchange the order of $A_i B_i$ and $\overline{A}_i B_i$.

4.2 Binary adder

Binary adder performs addition of binary numbers. The half-adder adds two single binary digits A_i and B_i, with two outputs sum S_i and carry C_i. The outputs can be expressed as:

$$\begin{aligned} S_i &= \overline{A}_i B_i + A_i \overline{B}_i = A_i \oplus B_i, \\ C_i &= A_i B_i. \end{aligned} \tag{3}$$

We combine AND gate and XOR gate in Figure 7 to realize half-adder in excitable medium. If carry C_i is put on the top of the structure of half-adder, the output channel of AND gate $A_i B_i$ should cross the channel $\overline{A}_i B_i$. A modified simple crossover is applied to achieve the function, since $A_i B_i$ and $\overline{A}_i B_i$ cannot be 1 at the same time. Figure 8 shows the structure of half-adder, where the crossover structure is marked by a box. Simulation results are shown in Figure 9 and Reference [23](videos). Table 1 lists all possible inputs and the corresponding outputs. It is found that the device realizes the addition of two bits.

A full-adder adds three one-bit numbers, including two single bits and the carry from the previous significant bit position. As shown in Figure 10, full-adder can be built by using two half-adders. Two bits A_i and B_i are added first, and then the sum of them is added to the carry C_{i-1} to generate the final sum S_i. The final carry C_i is produced by ORing carries of two half-adders.

FIGURE 9
Simulation results of half-adder when inputs (A_i and B_i) are (a) 1, 0. (b) 0, 1. (c) 1, 1.

It is easy to extend the basic adder units to multi-bit binary adders. An n-bit ($n \geqslant 2$) binary adder is constructed by combining a $(n-1)$-bit adder and a one-bit full adder. For example, Figure 11 shows the structure of three-bit binary adder. It consists of a one-bit full-adder (dashed box) and a two-bit binary adder (solid box), which also consists of a one-bit full-adder and a one-bit half-adder. Penetration units are used in the structure for pulse delay [22]. Figure 12 shows one of the simulation results. When inputs ($A_2A_1A_0$ and $B_2B_1B_0$) are 110 and 011, the corresponding output ($C_2S_2S_1S_0$) is 1001. All other simulation results of three-bit binary adder can be found in reference [23].

4.3 Binary encoder

Binary encoder compresses 2^n (or fewer) binary inputs into n outputs. The Boolean expressions of a two-bit (4 to 2) binary encoder can be represented as:

$$\begin{aligned} Y_1 &= I_2 + I_3, \\ Y_0 &= I_1 + I_3. \end{aligned} \tag{4}$$

Where I_3–I_0 are inputs, Y_1 and Y_0 are outputs. Moreover, a group signal (GS) is provided as an additional output for cascade. GS is asserted when one or

A_i	B_i	S_i	C_i
0	0	0	0
0	1	1	0
1	0	1	0
1	1	0	1

TABLE 1
Functionality of half-adder.

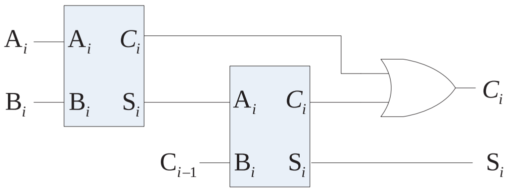


FIGURE 10
Block diagram of full-adder.

more of the inputs are active, which is expressed as:

$$GS = I_0 + I_1 + I_2 + I_3. \tag{5}$$

The related inputs are ORed to produce all three outputs. This device can be constructed based on OR gates and chemical diodes in excitable medium. In the simple case, we ignore the order of inputs and outputs in the structure.

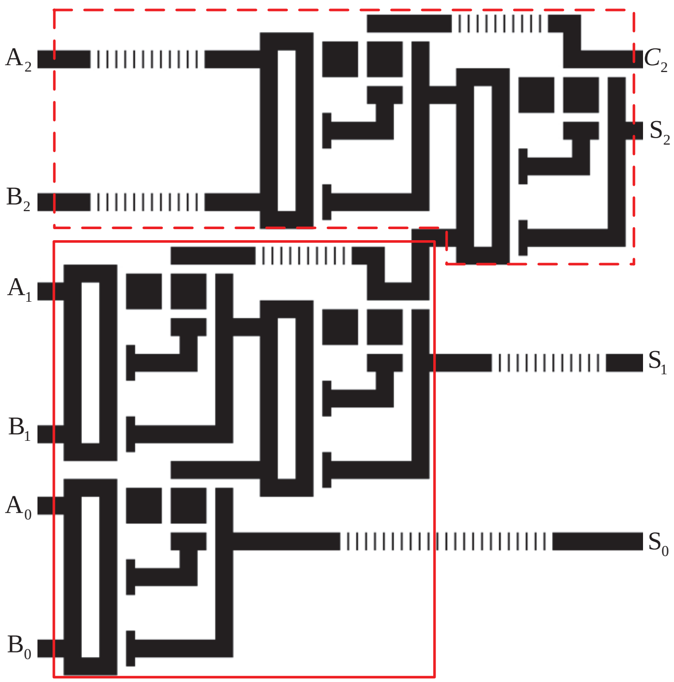


FIGURE 11
The structure of three-bit binary adder. This structure consists of a one-bit full-adder (dashed box) and a two-bit binary adder (solid box).

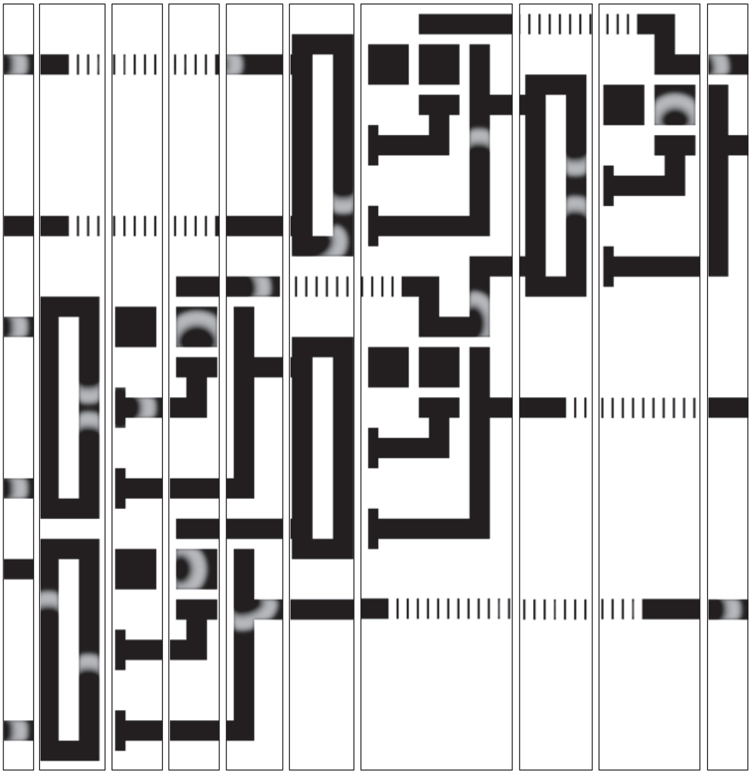


FIGURE 12
Simulation result of three-bit binary adder with inputs ($A_2A_1A_0$ and $B_2B_1B_0$) 110 and 011.The corresponding output ($C_2S_2S_1S_0$) is 1001.

In such a case, input channel I_3 is put between channel I_1 and I_2 to generate output Y_0 and Y_1 conveniently; furthermore, channel Y_0 and Y_1 intersect, so that the pulse from channel I_1 can propagate to channel GS. There will be only one crossover structure if the output channels intersect, while two crossover structures are needed for crossing of input channels (channel I_1 should cross I_2 and I_3). Since two input pulses never go through the crossover at the same time, and only one output pulse is sent at any given time, a simple crossover structure, which is marked by a box, is employed to achieve crossing, as shown in Figure 13.

Figure 14 shows the simulation results of two-bit binary encoder (corresponding videos can be found in reference [23]). When channel I_1 or I_2 has pulse (input is 0010 or 0100), a single pulse passes the crossover and generates the final outputs, as shown in Figure 14 (b) and (c). When channel I_3 has pulse (input is 1000), two pulses propagate into the crossover, as Y_0 and

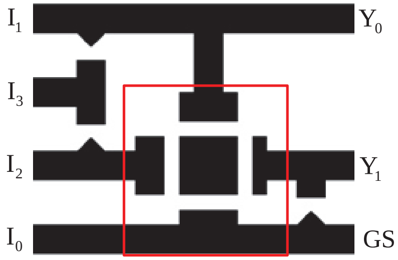


FIGURE 13
The structure of two-bit binary encoder. A simple crossover structure is used to exchange the order of Y_0 and Y_1.

Y_1 are both 1 at this time. The pulse from channel Y_1 arrives at the crossover earlier than the pulse from channel Y_0, as shown in Figure 14 (d), then the pulse from channel Y_0 cannot pass the crossover. As a result, there is still one output pulse in channel GS. Table 2 lists all possible inputs and the

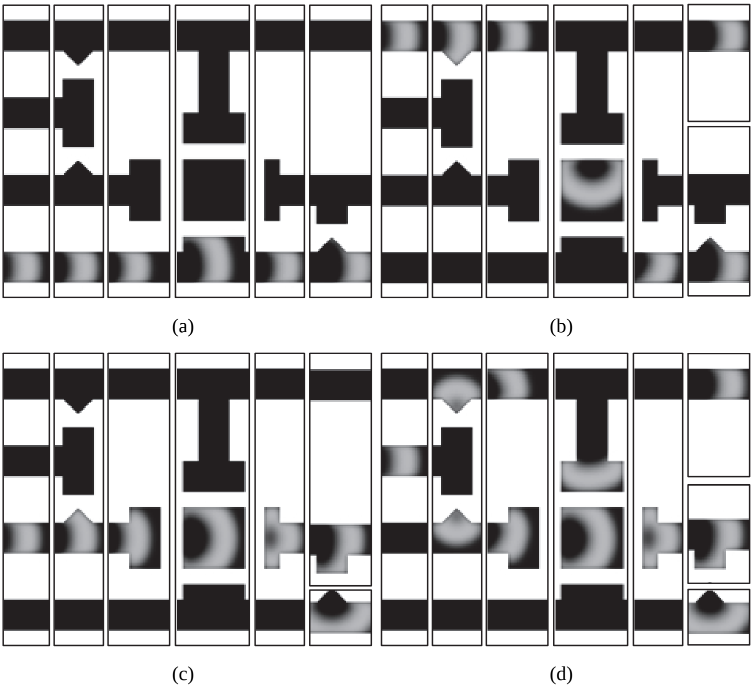


FIGURE 14
Simulation results of two-bit binary encoder when input $(I_3 I_2 I_1 I_0)$ is (a) 0001, (b) 0010, (c) 0100, (d) 1000.

I_3	I_2	I_1	I_0	Y_1	Y_0	GS
0	0	0	1	0	0	1
0	0	1	0	0	1	1
0	1	0	0	1	0	1
1	0	0	0	1	1	1

TABLE 2
Functionality of two-bit binary encoder.

corresponding outputs. It is clear that this device implement information encoding of two bits.

Note that the inputs and outputs are not arranged in order in Figure 13. We do not add more crossovers to make them in order for simplicity.

Multi-bit binary encoders can be formed from the basic encoders. An n-bit ($n \geqslant 2$) binary encoder is constructed by cascading two $(n-1)$-bit encoders. For example, Figure 15 shows the block diagram of three-bit (8 to 3) binary encoder, which includes two two-bit binary encoders. The outputs of the individual two-bit encoders are ORed to produce Y_0, Y_1 and GS, respectively, and GS of the higher encoder is regarded as output Y_2. There are three crossovers in Figure 15, which are marked by circles. The structure of three-bit binary encoder is shown in Figure 16, where three additional simple crossover structures are introduced to produce the final outputs. Figure 17 shows one of the simulation results. When input ($I_7 I_6 I_5 I_4 I_3 I_2 I_1 I_0$)) is 1000000, the corresponding output ($GS\ Y_2 Y_1 Y_0$) is 1111. Simulation results with all other inputs can be found in reference [23].

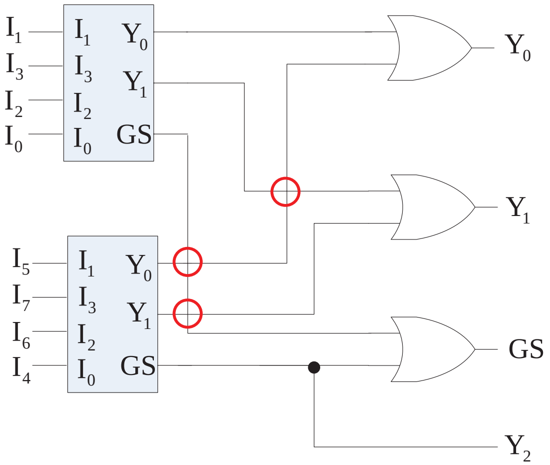


FIGURE 15
Block diagram of three-bit binary encoder. The crossovers are marked by circles.

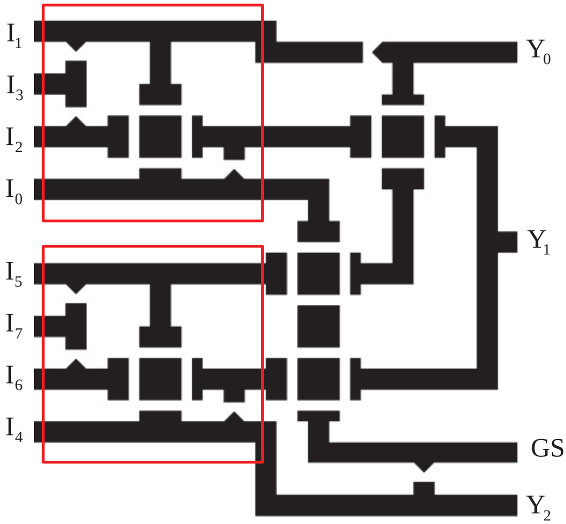


FIGURE 16
The structure of three-bit binary encoder. This structure consists of two two-bit binary encoders (marked by boxes) and three additional simple crossover structures.

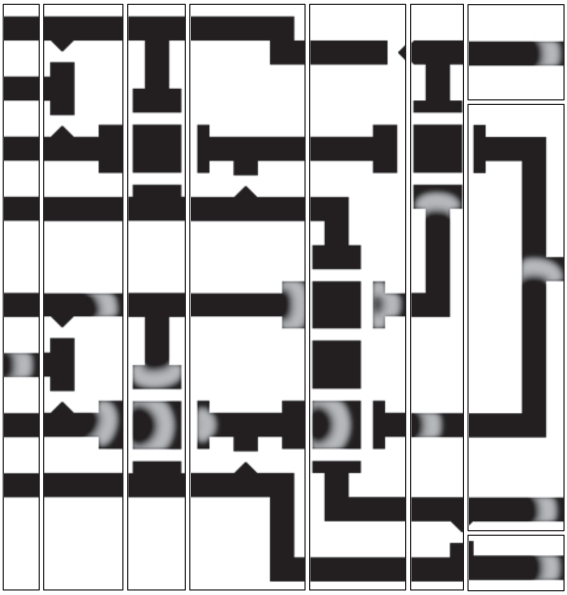


FIGURE 17
Simulation result of three-bit binary encoder with input ($I_7 I_6 I_5 I_4 I_3 I_2 I_1 I_0$) 1000000. The corresponding output ($GS\ Y_2 Y_1 Y_0$) is 1111.

4.4 Binary decoder

A decoder is a digital circuit that performs the inverse operation of an encoder. It has n input lines and a maximum of 2^n unique output lines. Reference [22] designed and implemented a kind of multi-bit binary decoder based on the BZ reaction. The structures occupy little space, but need careful design for strict synchronization of the pulses. In this paper, we will show another way to construct higher-bit binary decoders by cascading lower-bit binary decoders directly.

The logic expressions of one-bit (1 to 2) binary decoder are given by Equation (6), where I_0 is the input, and Y_1, Y_0 are outputs. Similar to reference [22], one-bit binary decoder is built by combining AND gate and NOT (AND NOT) gate with an auxiliary 1 input. Figure 18 shows the structure, in which the auxiliary 1 input is put at the bottom.

$$\begin{aligned} Y_1 &= I_0 = I_0 1, \\ Y_0 &= \overline{I_0} = \overline{I_0} 1. \end{aligned} \tag{6}$$

Similar to binary encoders, we can form multi-bit binary decoders from the basic decoders. An n-bit ($n \geqslant 2$) binary decoder is constructed by cascading two $(n-1)$-bit decoders. For example, Figure 19 shows the block diagram of two-bit (2 to 4) binary decoder. The auxiliary 1 inputs of both one-bit decoders originate from I_1, which acts as a selector between the two decoders. It allows I_1 to enable either higher or lower decoder, which produces outputs Y_3, Y_2 or outputs Y_1, Y_0. We should exchange the order of I_0 and I_1 ,as shown in Figure 19. A multi-functional crossover structure is involved, as pulses from channel I_0 and I_1 may appear simultaneously. Figure 20 illustrates the structure of two-bit binary decoder, which includes two one-bit decoders (solid boxes), a crossover structure (dashed box) and

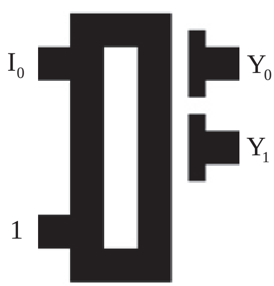


FIGURE 18
The structure of one-bit binary decoder.

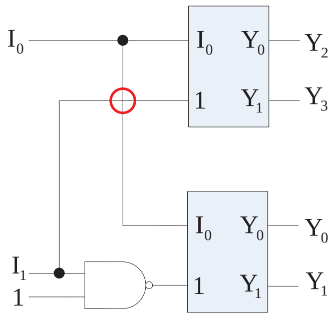


FIGURE 19
Block diagram of two-bit binary decoder. The crossover is marked by a circle.

a NOT gate. Chemical diodes are introduced to prevent the interactions of the inputs. Figure 21 shows one of the simulation results. When input ($I_1 I_0$) is 11, the corresponding output ($Y_3 Y_2 Y_1 Y_0$) is 1000. Simulation results with other inputs can be found in reference [23].

5 CONCLUSION

It is very important to achieve the function of crossing wires in the BZ excitable medium due to the planar restriction of the channel structures.

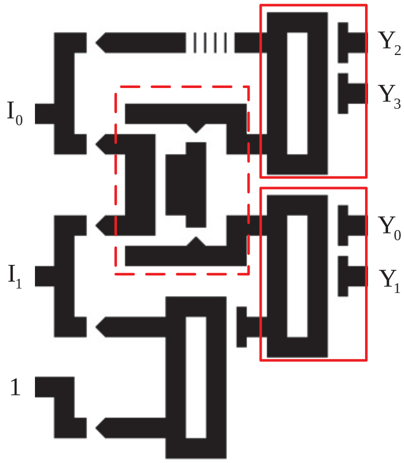


FIGURE 20
The structure of two-bit binary decoder. This structure includes two one-bit decoders (solid boxes), a multi-functional crossover structure (dashed box) and a NOT gate.

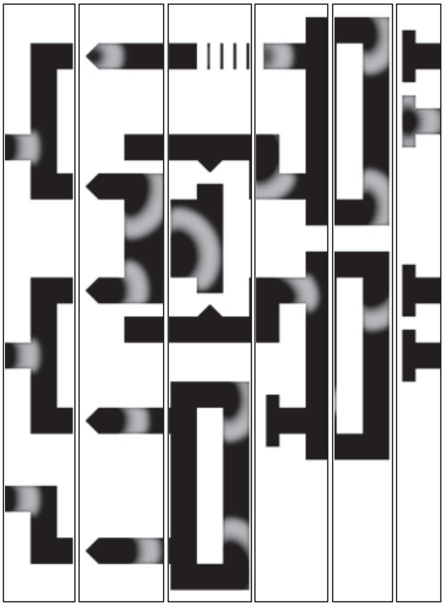


FIGURE 21
Simulation result of two-bit binary decoder with input ($I_1 I_0$) 11. The corresponding output ($Y_3 Y_2 Y_1 Y_0$) is 1000.

In this paper, we designed and implemented two kinds of crossover structures in simulation based on the BZ reaction. One has simple structure, and realizes single input single output cross propagation by the property of angle dependent penetration. The other is complex and powerful. This structure, which is built with chemical diode, T-shaped coincidence detector and angle dependent penetration unit, permits two inputs to propagate highly or nearly simultaneously and keeps two outputs synchronized. Furthermore, the crossover structures are applied to design combinational logic circuits. We constructed and implemented, through simulations, multi-bit binary adder, multi-bit binary encoder and multi-bit binary decoder by cascading method, which is similar to the method in digital electronics.

The crossover structures and the combinational logic devices are constructed using only the existing elements, such as straight channel, chemical diode, T-shaped structure and penetration structure, which have already been verified in experiments. Therefore, we believe that these devices can be implemented in excitable medium. However, due to the uncertainties of chemical experiments, we should pay attention to the synchronization of the input pulses in T-shaped structures and proper width of the stripe in penetration structures, thus, these devices can work well.

Crossover structures are commonly used in digital electronics. In this paper, the crossover structures we designed are simple and effective. They expand the function of logical computations based on the BZ reaction and can be used as elements of more complex devices. Next, we will use the crossover structures to construct flip-flop, which is the basic storage element in sequential logic. Moreover, other sequential logic devices, such as counter, memory, can be implemented, guiding to the construction of chemical computer.

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