The Relation between Wave Velocity and Thickness of the System about the B-Z Reaction

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1 Abstract

There are a lot of beautiful patterns with good symmetry in this world, specially in the biological world, such as spirals of the shells, rings in a tree, fractals of branches, etc. The second law of thermodynamics says that entropy increases in the closed system. Therefore, this patterning cannot be explained as a closed system. It is not explained until taken as unequilibrium open system. However, the theory of unequilibrium system is much more complexed than that of closed system. Happily, we know the Belosov-Zhabotinskii reaction (B-Z reaction). It can be easily experimented, but stands for unequilibrium open system.

I used the B-Z solution system and examined how the wave velocity changes with different thickness of the system. Then, I observed what phenomenon happens when the thickness is different according to the position. The results were compared with the two simulations. One is based on the diffusion equation; the other is based on the cellular automaton model.

2 Method and Result

2.1 Preparation

I used the B-Z solution system shown as follows:

$NaBrO_3$	0.45 M
H_2SO_4	0.36 M
Maronic Acid $((CH_2COOH)_2)$	0.20 M
KBr	0.050 M
Ferroin $([Fe(phen)_3]^{2+})$	0.0020 M

Moreover, I put tween 20, non-ionic surfactant, into the solution in order not to reduce the influence of meniscus.

2.2 The Wave Velocity against Thickness of the System

I put the chemicals into a petri dish. I varied the total quantity. After putting a pace-maker into the solution, I recorded the patterns with a video camera. With a computer, I measured the time and position of some wave fronts of target patterns. From the data, the velocity was calculated. The wave velocity against thickness is shown in Fig.1.

Fig.1 shows that the thicker the system is, the faster the wave velocity is. I calculated that the correlation function is 0.69, which shows wave velocity and thickness has positive correlation. By the way, when the thickness is 0.52 mm, waves did not propagate. So, I defined that the velocity at 0.52 mm is 0.

2.3 The Phenomenon in the Inclined System

The petri dish with 3-mlsolution (If put horizontally, the thickness is 0.52 mm.) was inclined. (One side of the petri dish with a radius of 43 mm is about 1 mm higher than the other.) Then, waves generated in the thicker

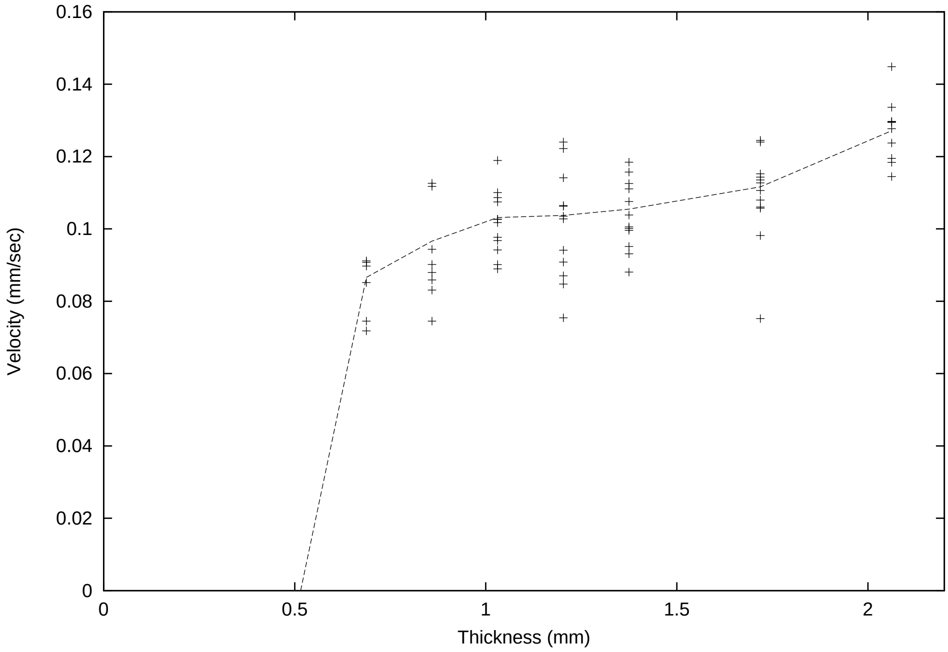

Figure 1: The velocity of the wave fronts against the thickness of the system. The line is the avarage velocity. The points are the wave velocity of each wave front.

area and propagated to the thinner area. As the waves propagated to the thinner area, wave velocity decreased. The following wave caught up with the before one, and disappered.

I measured the relation between time and position of each wave front, and plotted it. The result is shown in Fig.2.

3 Simulation

3.1 The Model using Diffusion Equation

3.1.1 Mechanism

The diffusion equation :

$$\frac{\partial f}{\partial t} - \kappa \nabla^2 f = 0 \quad \text{with} \quad \kappa = 1\,, \quad f(\vec{x}, 0) = \delta(\vec{x}) \tag{1}$$

has a solution as follows:

$$f(\vec{x}, t) = \left(\frac{1}{4\pi t}\right)^{\frac{3}{2}} \exp\left(-\frac{|\vec{x}|^2}{4t}\right) \tag{2}$$

Now, I assume three things:

1. The activator diffused from the wave front. Wave propagation is only due to this cause.
2. Wave front is a plain. From every point on the plain, the activator independently diffused as the diffusion equation descrides.
3. A place becomes wave front when the sum of the activator reaches a certain threshold.

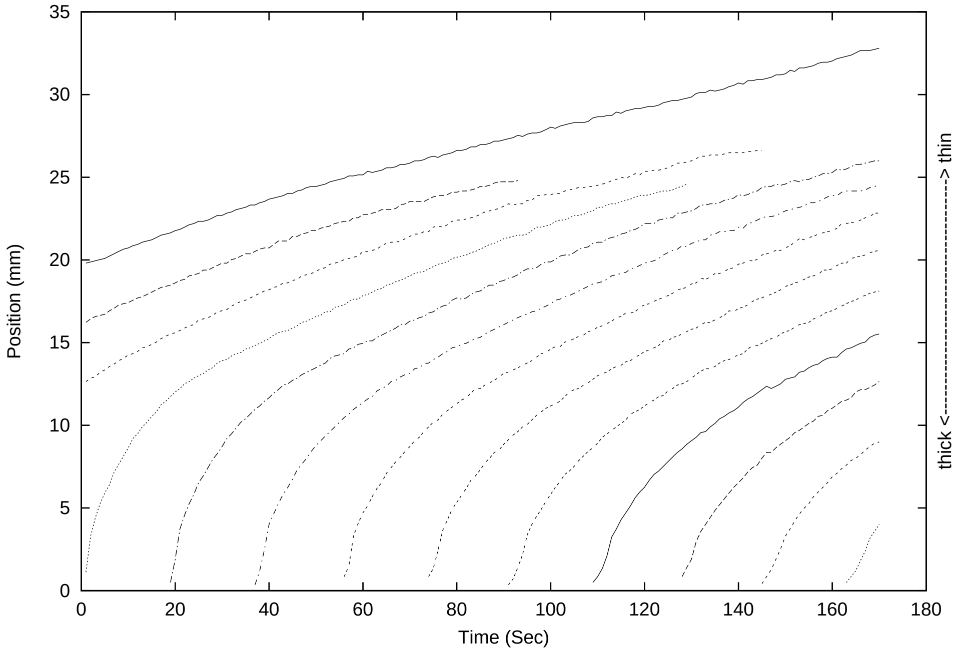

Figure 2: The wave propagating from the thicker area to the thinner area. Three wave fronts disappears as they catch up with another wave.

In this system, BrO_3^- is the activator. Based on the assumption, I watch the position in front of the wave front by length l. Suppose that the depth is d, and that the threshold is $f_{\rm th}$ (See Fig.3). Then $t_{\rm th}(d)$ is got which satisfys the equation as follows:

$$\begin{aligned} f_{\rm th} &= \int_{-\infty}^{\infty} dy \int_{-\frac{d}{2}}^{\frac{d}{2}} dz f((l,y,z),t_{\rm th}) \\ &= \frac{1}{4\pi t}\int_{-\frac{d}{2}}^{\frac{d}{2}} dz \exp\left(-\frac{l^2+z^2}{4t}\right) \end{aligned} \tag{3}$$

To make things easier, t and $f_{\rm th}$ is defined again: $4t \longrightarrow t$, $\pi f_{\rm th} \longrightarrow f_{\rm th}$.

$$f_{\rm th} = \frac{1}{t}\int_{-\frac{d}{2}}^{\frac{d}{2}} dz \exp\left(-\frac{l^2+z^2}{t}\right) \tag{4}$$

The equation (4) is used with the simulation.

3.1.2 The Result of the Simulation and Comparison

I got the relation between $t_{\rm th}$ and d. As $v = l/t_{\rm th}$, velocity v against thickness d is known. It is plotted in Fig.4

From this simulation, there is a thickness (critical thickness) at which wave velocity becomes slow and wave does not propagate. The experiment also showed the exisitence of a critical thickness. When the system is thick, the simulation shows that the wave velocity has a limit. However, I could not observed this characterisitics. I should increase the quantity of the solution, but as the system becomes thick, three-dimensional structures prevent from accurate measurement.

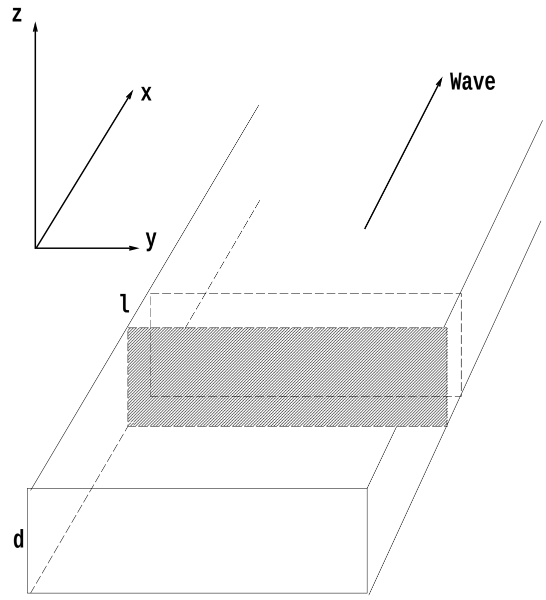

Figure 3: Mechanism

3.2 The Model with the Cellular Automaton

3.2.1 Mechanism

Cellular automaton is one of the models that stands for B-Z reaction. The followings are assumed:

1. The system is devided into some cells whichare influenced only by the next cells.
2. Each cell is in either of the three state: excited state `@`, dead state `o`, ground state `-`.
3. A cell in the excited state turns into the dead state in a certain span.
4. A cell in the dead state turns into the ground state in a cetrtain span.
5. A cell in the ground state turns into the excited state in a certain span only if any next cells are in the excited state.

Based on the assumptions, initial conditions and boundary conditions decide the wave propagation. Generally, the wave velocity is thought to be constant. This means that the span is independent of the position. Now, I supposed that the span is dependent on the position; The span in which a cell in the excited state turns into the dead state depends on the position. A cell in the ground state turns into the excited state, when next cells turn into the dead state. The span in which a cell in the dead state turns into the ground state is independent of the position.

3.2.2 The results of the Simulation and Comparison

The result of the simulation is shown in Fig.5. It shows a phenomenon like this: At the Thicker area, two waves have enough interval and exist independently. However, as they propagate to the thinner area, they come close and one disappears. This phenomenon accords with the result of the experiment.

4 Discussion and Problem

About the experiment of the relation between two wave velocity and thickness, there are some problems. One is that the influence of meniscus cannot be ignored, specially when the system is thin. In fact, the phenomenon

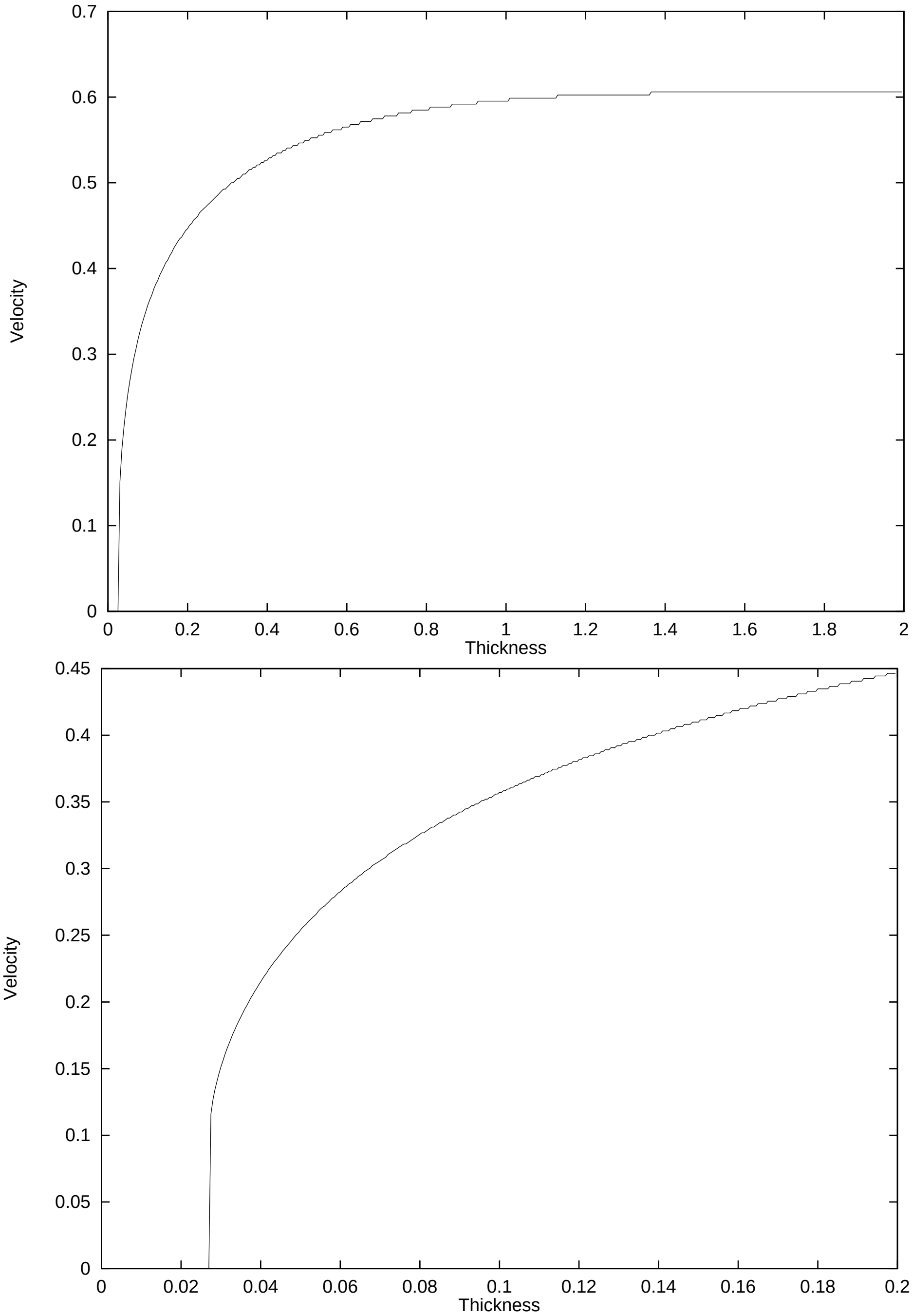

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Figure 4: The result of the simulation using the diffusion equation. Now, $l = 0.1$, $f_{\rm th} = 0.01$. The area where d is small in the upper figure is shown in the lower figure.

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Figure 5: The result of the simulation using the cellular automaton model. The left side is thick and the right side is thin. One wave catches up with another wave and disappears.

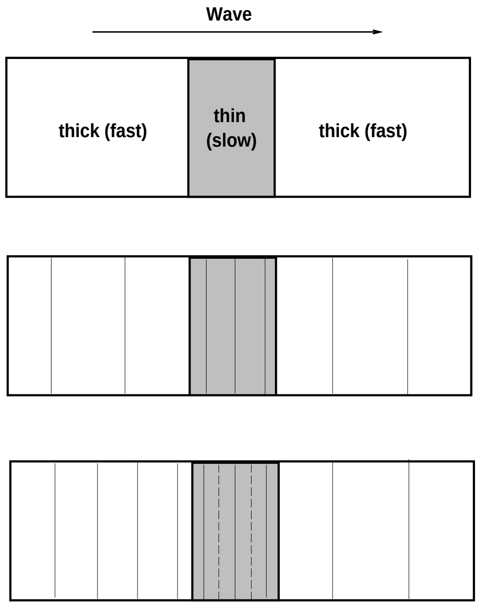

Figure 6: The application to the filter. In the meshed area, the wave velocity is slow. When waves propagate from left to right, the long-periodic waves propagates, but some of the short-periodic waves disappears.

was observed that at the edge of the petri dish waves could propagate, but that at the center they could not. In the experiment, I put the pacemaker at almost the same position, but it is not perfect. If I use the system of gel, this problem will be solved. However, the system of solution may be different from that of gel. The other is when the system is thick enough for three-dimensional structures. Owing to these problems, the model using diffusion equation cannot be judged right or wrong.

The penomenon that a wave catches up with the other wave and disappear seems expalined as follows: The wave front is oxidation wave, so Fe^{3+} increases there. After oxidated rapidly, Fe^{3+} is slowly reduced into Fe^{2+} by increasing inhibitor (Br^-). By the way, if the interval of waves are short, the oxidation wave comes while the inhibitor increases. Then, inhibitor prevents Fe^{3+} from generating. This means that the catching-up wave does not propagate any longer and disappears. The celular automaton model is based on the idea of the activator and inhibitor. The result of simulation and experiment is alomst the same, so the discussion above seems to be vaid.

This penomenon is very interesting and can be applied. When waves propagate from the thinner area to the thicker area, every wave prpopagates. On the contrary, when they propagate from the thicker area to the thinner area, some waves may disappear if the period is short. Using this phenomenon a kind of element can be made. For example, when wave velocity is slow at one area, this element is a kind of filter. If the period is long, the waves propagate without any influence, but if the period is short, some waves disappeared and the period of the output waves is more than a certain time. (See Fig.6)

5 Conclusion

From the experiment and simulation, the following can be concluded:

1. The wave velocity is faster, as the system thicker.
2. The wave velocity does not propagate, when the system is thinner than a critical thickness.
3. The series of the waves propagating from the thicker area to the thinner area are observed. The following wave catches up with the before one, and disappears.

4. Both of the simulation using the diffusion equation and the cellular automaton are fit with the result of experiment to some extent.

6 Acknowledgement

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