Models of reaction-diffusion systems

Chemically-Generated Letters

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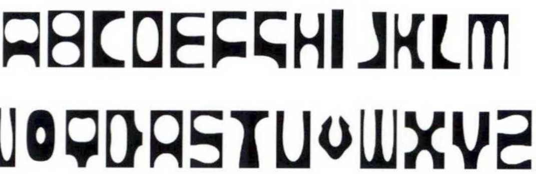
One of the most fascinating problems in contemporary science is the generation of shapes and patterns in biological systems

Our visible world is composed of various shapes. Some of them are very regular (symmetrical), and therefore easy to remember. Others are irregular but nevertheless easy to remember and distinguish, like children's faces for their parents. Sill others are irregular and very difficult to remember, like the shapes of clouds. Shapes of all these kinds are spontaneously generated by nature. In addition, we are also surrounded by a variety of shapes produced by human activity, usually described as "artificial." However, this characterisation is not completely correct, because such shapes are also produced by biological systems, according to the laws of nature. Thus, the question how biological systems can generate supposedly "artificial" shapes is one of the most fascinating aspects of contemporary science.

Alan Turing was a pioneer in explaining the generation of shapes in biological systems on the most fundamental level. In 1952, he showed that the model of a one-dimensional (1D) system in which only the appropriate chemical reactions and diffusion occur had asymptotic solutions that were stationary but periodical in space. Now, reaction-diffusion systems can be treated as the minimal models for various patterns observed in biology, and more generally in nature. They are useful models for explaining the generation of so-called positional information, which determines the differentiation processes of living cells during the growth of an organism.



The set of asymptotic patterns generated in twenty six 2D systems. These patterns were obtained in rectangles of different sizes and different initial conditions, and have been slightly deformed to give the letters approximate height and width. All letters are formed from the patterns by separating the asymptotic values of the reactant distribution into two regions, with values of the reactant higher (or lower) than some arbitrary number. One of these two regions is marked in black

The set of asymptotic patterns generated in twenty 2D systems. These patterns were obtained in convex or concave systems with different sizes and initial conditions, and have been slightly deformed to give the Old Hebrew letters approximate height and width

Real nonlinear reaction-diffusion systems provide useful caricatures of many biological systems. For example, running waves can be easily observed experimentally in a thin layer of reaction mixture in which the Belousov-Zhabotinsky (B-Z) reaction occurs (the oxidation of various organic compounds by bromate ions in presence of catalysts). They can be seen as expanding blue rings on a red solution, if the proper concentrations of bromate, bromomalonic acid, ferroine and sulfuric acid are used as the B-Z reactants. The qualitative properties of such waves are similar to the spreading of electrical excitations along axons in neurons, as well as to waves in the Purkinje fibers in the heart. Let us mention that it is much easier to investigate the qualitative properties of such waves in chemical systems than in biological ones.

Asymptotic solutions to excitable reaction-diffusion equations in two dimensional (2D) systems with appropriate initial and boundary conditions can also take the form of stationary but spatially periodical distributions of reagent concentrations. Such distributions have been observed in experiments performed in 2D continuously-fed unstirred reactors (2D CFURs). Experiments and models of reaction-diffusion systems enrich our knowledge about the possibilities for generating various patterns on the physicochemical level. Several quite natural questions arise here: How rich is the variety of patterns generated by reaction-diffusion systems? Can we construct models whose solutions exhibit certain desired distributions? The answers to these questions are partially positive.

In order to show examples illustrating the richness of the possible patterns, a model of an excitable reaction--diffusion system has been developed, whose asymptotic solutions have forms mimicking all the capital letters of both the Latin alphabet and the Old Hebrew alphabet. The model consists of two coupled catalytic (enzymatic) reactions. One of them is allosterically inhibited by an excess of its reactant and product. The other one is a usual catalytic (enzymatic) reaction, which proceeds in its saturation regime. These reactions are assumed to occur in an open system, i. e. 2D CFURs with boundaries impermeable to the reagents. The conditions under which such virtual experiments were performed were identical for all letters in both alphabets, meaning that all parameters in the reaction-diffusion equations were the same. Only the sizes of the reactor and the locations of initial excitations have to be changed to generate the desired patterns. All the capital Latin letters can be obtained in reactors with concave areas, whereas some Old Hebrew letters can be generated in the reactors with concave shapes (rectangular polygons with 6, 8 or 10 apexes). For simplicity all numerical calculations have been performed for 2D CFURs in the form of rectangles (for the Latin alphabet) or rectangular polygons (some Old Hebrew letters). The results of calculations are presented in Figs. 1 and 2. The contours of all letters visible on these Figs have been obtained by separating the asymptotic solutions into two regions. The regions in which the concentration of the reactant is higher than some selected value are marked in black.

Not all letters have elegant forms. Some of them resemble scribbling, but they are indeed readable, especially when used in sets meaning words. More elegant forms of the letters can be obtained if one uses reactors with smooth boundaries instead of rectangular polygons. It is noteworthy that the reaction-diffusion model is structurally stable, which means that small changes in its parameters do not change the shapes of the asymptotic solutions. Moreover, small changes in the sizes of the reactors and positions of initial excitations do not change the qualitative properties of the asymptotic solutions.

All the letters have been obtained as asymptotic solutions of the deterministic problem with well defined inhomogeneities as the initial distributions of reagents. In real systems inhomogeneities can appear due to internal, local fluctuations. There is, therefore, a greater-than-zero probability that the patterns might appear spontaneously in real systems. It is noteworthy that the model is not an exceptional one. Identical patterns can be generated in many reaction-diffusion systems, provided they have qualitative properties similar to the presented model. Moreover, it is worth stressing that the model contains only two variables, and is therefore a simple one. We can expect richer patterns in systems with three, four and more variables.

The nonlinearities governing the chemical dynamics in the model presented in this paper are often found in many-variable models which are usually used to describe real chemical systems. Therefore, one can expect that in the future nonlinear chemical systems may serve as tools for the self-generation of two-dimensional patterns with desired shapes. ■

Further reading:

Turing A. (1952). The chemical basis of morphogenesis, *Philos. Trans. Roy. Soc. London, B 237*, 37.

Kawczyński A. L., Legawiec B. (2001). A two-dimensional model of reaction-diffusion system as a typewriter. *Phys. Rev. E, 64*, 056202-1.

Kawczyński A. L., Legawiec B. (2004). A two-dimensional model of reaction-diffusion system as a generator of Old-Hebrew letters. *Polish J. Chem., 78*, 733.

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Spontaneous pattern formation in the Belousov-Zhabotinsky reaction resambles a target and is known as the target pattern