MULTIPLICITY OF STATIONARY PATTERNS IN AN ARRAY OF CHEMICAL OSCILLATORS

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It is shown that at least a few hundred stationary patterns may be found in a 1-dimensional array of chemical oscillators described by the Brusselator model. During conducted calculations all system parameters were kept constant and only responses of chemical system to perturbations were the subject of studies. The developed patterns are characterized by sharp maxima in concentrations of species U separated by areas of low concentrations. The questions how many patterns are possible and how are they organized are still the subject of study , however the following properties have been established:

a) Concentration of a component U as a function of the amplitude of perturbation forms a staircase diagram.

b) Maxima in concentrations of component U may be obtained in any place in the system.

c) Distances between two maxima have an upper limit, however; below this limit any distance is possible.

These fascinating spatial chemical structures are the subject of detailed studies which will be reported in the coming paper.

Introduction

Biological morphogenesis - development of complex organism from a single cell is probably the most mysterious and fascinating phenomenon in the universe. However development of forms is not exclusive to biological phenomena, but can also be observed in chemical, physical and geological systems. These fascinating structures attracted the brightest minds of the twentieth century such us (J. von Neuman 1966), (A. Turing 1952) or (S. Ulam 1976). Developed by J. von Neuman and S. Ulam the cellular automata theory shown that the incredible reaches of forms and even behaviors can be observed when simple elements interact together. Furthermore, the paper by A. Turing shows that the interaction of diffusion and chemical kinetics may lead to the formation of chemical structures where the concentrations of chemical species are organized in space. This fascinating idea by A. Turing was explored by many biologists and chemists.

At the same time the pioneering works of I. Prigogine and G. Nicolis (I.Prigogine, G. Nicolis 1977) on dissipative structures, the discovery of chaos, chemical oscillations and chemical waves revolutionized modern science. The last ten years were very fruitful in discoveries in the field of nonlinear dynamics especially in chemical systems. However, the experimental realization of Turing structures has been achieved only recently (V. Castels, E.Dulose, J. Boissonade 1990).

Alongside with the experimental efforts in obtaining stationary chemical patterns, many theoretical works have also been done. Most of numerical calculations were oriented toward finding necessary conditions for developing Turing structures, searching for structure in known models of oscillatory chemical systems, and modelling experimental results. However, the theory of Turing patterns has not developed substantially beyond the pioneering work of Turing and later by the works of the Brussels group (M. Herschkowitz-Kaufman, G. Nicolis 1972) (M. Herschkowitz-Kaufman 1975) . Turing theory deals with the spontaneous transition from an uniform stationary pattern to a stable structure when concentrations are nonuniform in space. This theory describes phenomena only in vicinity of the bifurcation point and can not describe patterns which develop far from the bifurcation. Therefore the following important questions can not be answered;

1. How many patterns are possible in a given chemical systems?
2. What kinds of patterns are possible in chemical systems?
3. What will be the bifurcation diagram?
4. How will the transitions from one pattern to the other will be ordered by the bifurcation parameters?

There are not many theoretical papers dealing with these problems 9 D. Walgraef, D. Dewel, P. Borckmans 1980), (D. Walgraef, G. Dewel, P. Borcmans 1982), (J.Vostano, J.Pearson, W. Hosthemke, H.L. Swinney 1988). J. Vastano and H. Swinney have found, in a simple model of a chemical system, that only few patterns may exist simultaneously. They differ by the wave number. Most of patterns may not be reached by the Turing bifurcation but only by special perturbations. Therefore, the response of chemical medium to perturbations becomes the urgent issue. In this paper we will discuss in detail the problem of the response of chemical media to the perturbation and the relation between perturbations and developed structures.

Numerical calculations

The calculations in our laboratory have been conducted with the Brusselator as a model of an oscillatory chemical system. This model made it possible to conduct detailed studies of patterns in the case of sinusoidal-close to Hopf bifurcation chemical medium.
The Brusselator model is given by the following set of differential equations;

$dU/dt = A - (B+1)U+U^2V$

$dV/dt = BU - U^2V$

The following parameters were chosen for calculations:
$A=1.0$, $B=3.5$ D- diffusion coefficient for V componenet = $1x10^{-4}$, diffussion coefficient for U component is equal to zero. $L=0.20$, $N=100$ $dt= 0.001$ The explicit Euler method of integration was used with non-flux boundary conditions. Solutions are nonsensitive to time spacing but are sensiytive to spatial spacing. Therefore, this system should be treated as nonhomogenous similar to biological multicellular systems.

Results

a. Staircase diagram

In the first series of experiments, the response of chemical medium to perturbations with different amplitude was investigated. The uniform stationary state was perturbed in two central cells with different values of U. Developed patterns are presented in Fig.1. Obtained stationary structures have very similar shapes characterized by five maxima, however the concentrations of species U in maxima are different. The detailed diagram representing the concentrations in a central cell as a function of perturbation is shown in Fig.2a, whereas Fig.2b and Fig.2c represent magnified parts of Fig.2a. These diagrams exhibit a staircase similar to the staircase which is obtained during the study of a phase locking phenomena. However, between the steps, the typical self-repeating structures have not been found. In the range of perturbation from 0.1 to 0.3 developed patterns have very low concentrations of component U in the central cell. These patterns are characterized by four maxima and are presented in Fig.3. Similarly to the patterns with five maxima these patterns have comparable shapes however concentrations in maxima are different as well as positions of maxima are slightly shifted.

b. Memory effect

When the system was perturbed with the perturbation $U=5.0$ at different places in the space, then a new and interesting phenomenon has been discovered. The maxima of concentrations of species U in developed patterns were found in places of initial perturbations. The pattern which developed after cell 50 was perturbed is presented in Fig. 4a and patterns which developed after cells 74 or 89 were perturbed are presented in Fig. 4b and Fig.4c respectively. The developed patterns have four or five maxima and are similar to patterns discussed above, however, the chemical system actually "remembers" the position of the initial perturbation.

This interesting phenomenon was studied more carefully and obtained results are presented in Fig.5. The X- axis represents the dimensional space (100) cells. Dots represent maxima in developed stationary patterns. The Y-axis represents points of initial perturbations. The first row from the top corresponds to a pattern which developed after the cell 1 (first from the left) was perturbed. The second row represents pattern which developed after the cell 2 was perturbed. The diagonal line indicates that developed patterns always have the maximum in the position of the initial perturbation. When the position of the perturbed cell changes so do the positions of all maxima. However, the distance between maxima is preserved. A maximum which is shifted to the right, reaches the boundary and disappears. At the same time the new maximum is formed on the left side and the wavelength is preserved.

c. Separation of maxima

In the next computer experiment the system was perturbed in two places. The results are presented in Fig.6a. The distance between perturbation points increases from top to bottom. From the centrum of Fig.6a it is obvious that any distance between two maxima may be obtained if it is less than the characteristic wavelength. The example of chemical patterns with many maxima and different wavelengths is presented in Fig.6b. During our initial calculations, few hundreds of stationary patterns have been found. There are the subject of a detailed study which will be published in the coming paper.

Conclusion

The stationary chemical pattern discovered by us can not be described by the linear Turing bifurcation theory. Similarly, the Hopf bifurcation can not predict or describe the complex oscillations or chaotic attractors which may appear in dynamical systems. Therefore we may assume that many new and complicated patterns will be discovered during the numerical investigations of chemical stationary patterns. The structure presented in Fig.5 has a very unusual property. We may observe smooth transition from one pattern to the other. It is similar to toroidal oscillations where by continuously changing of initial conditions, oscillations slightly shifted in phase may be obtained. If we assume that the 1-D stationary pattern may be represented by the 1-D attractor then the structures discussed above should be presented as the 2-D attractor. The staircase diagram in Fig.2 suggests some relation with the high dimensional torus. It should not be surprising because 100 interacting oscillators may be described by a high dimensional torus. Therefore during the transition from torus to Turing patterns many new surprising structures may be observed.

Literature

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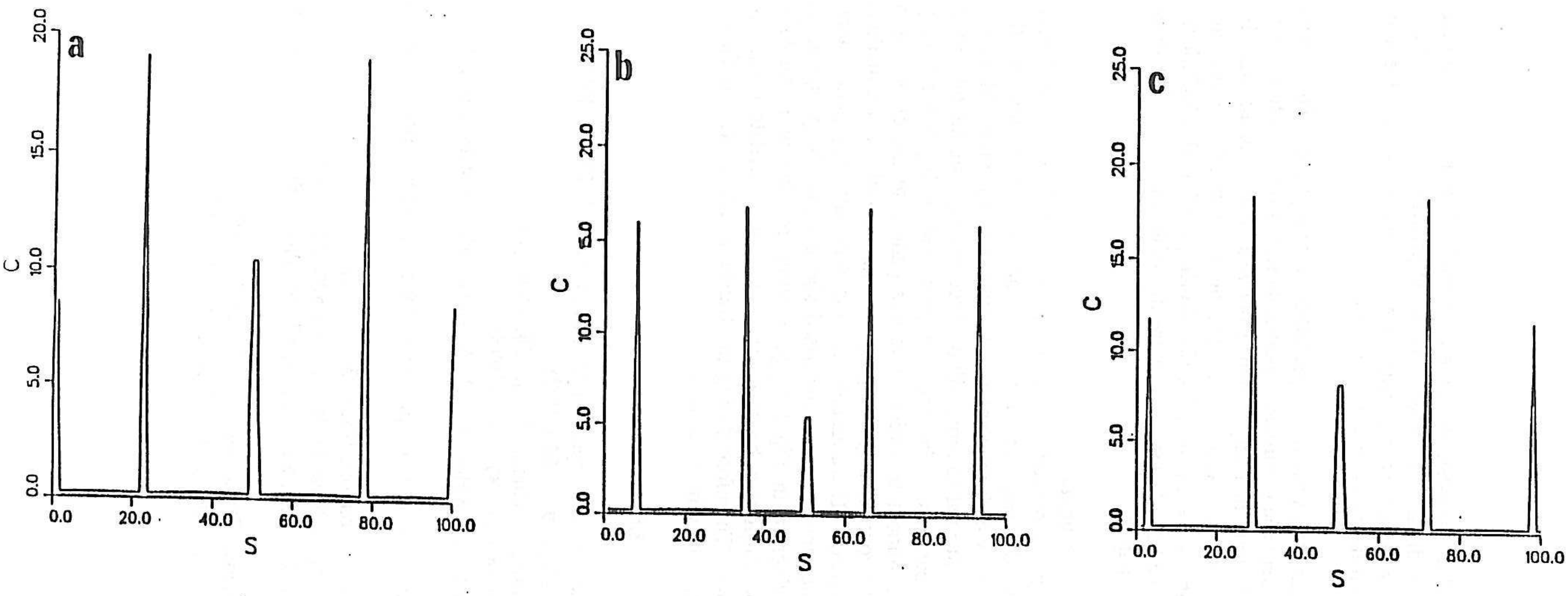
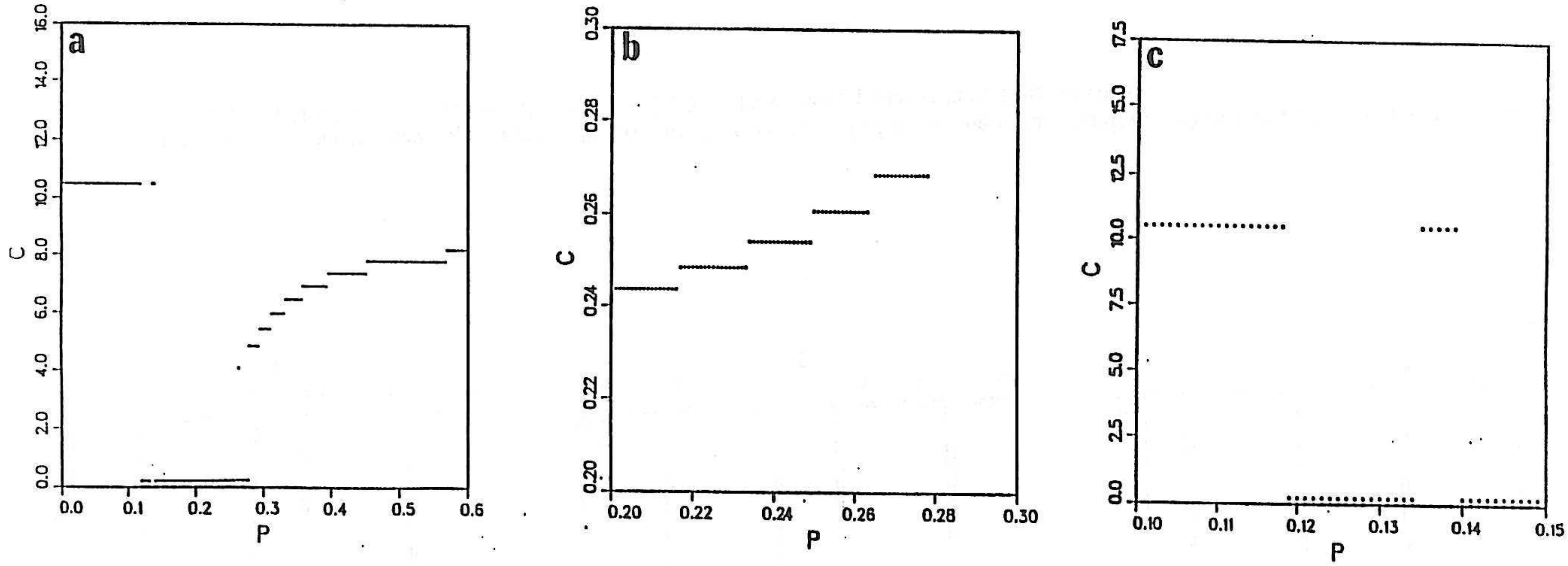
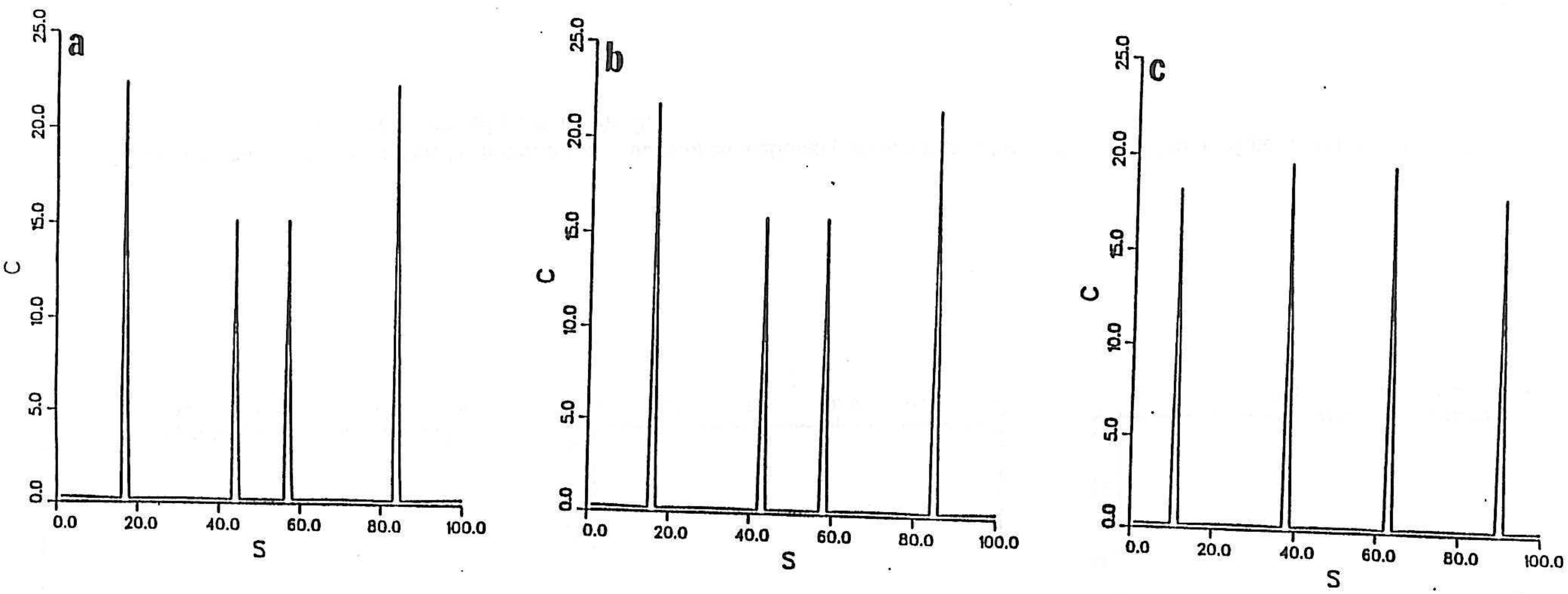


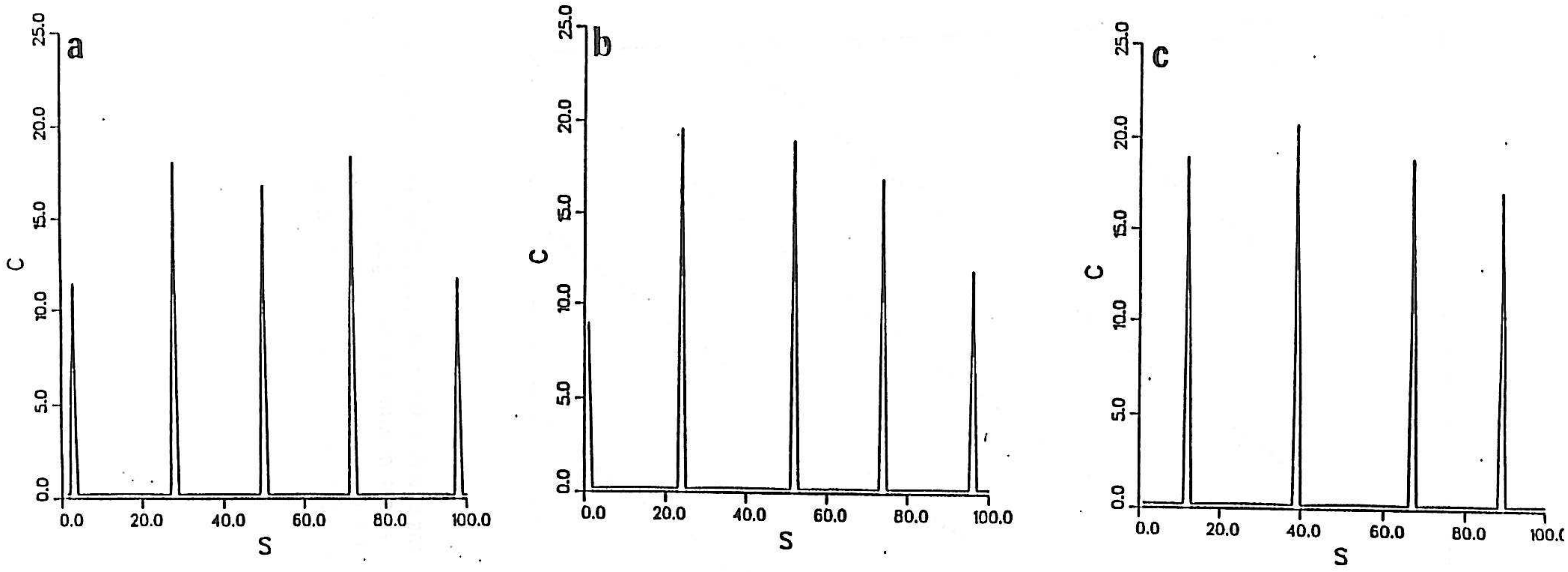
1. Stationary pattern developed after the cells 50 and 51 were perturbed by single perturbation. a) perturbation U = 0.05, b) perturbation U=0.3, c) perturbation U=0.6. Developed patterns have 5 maxima.



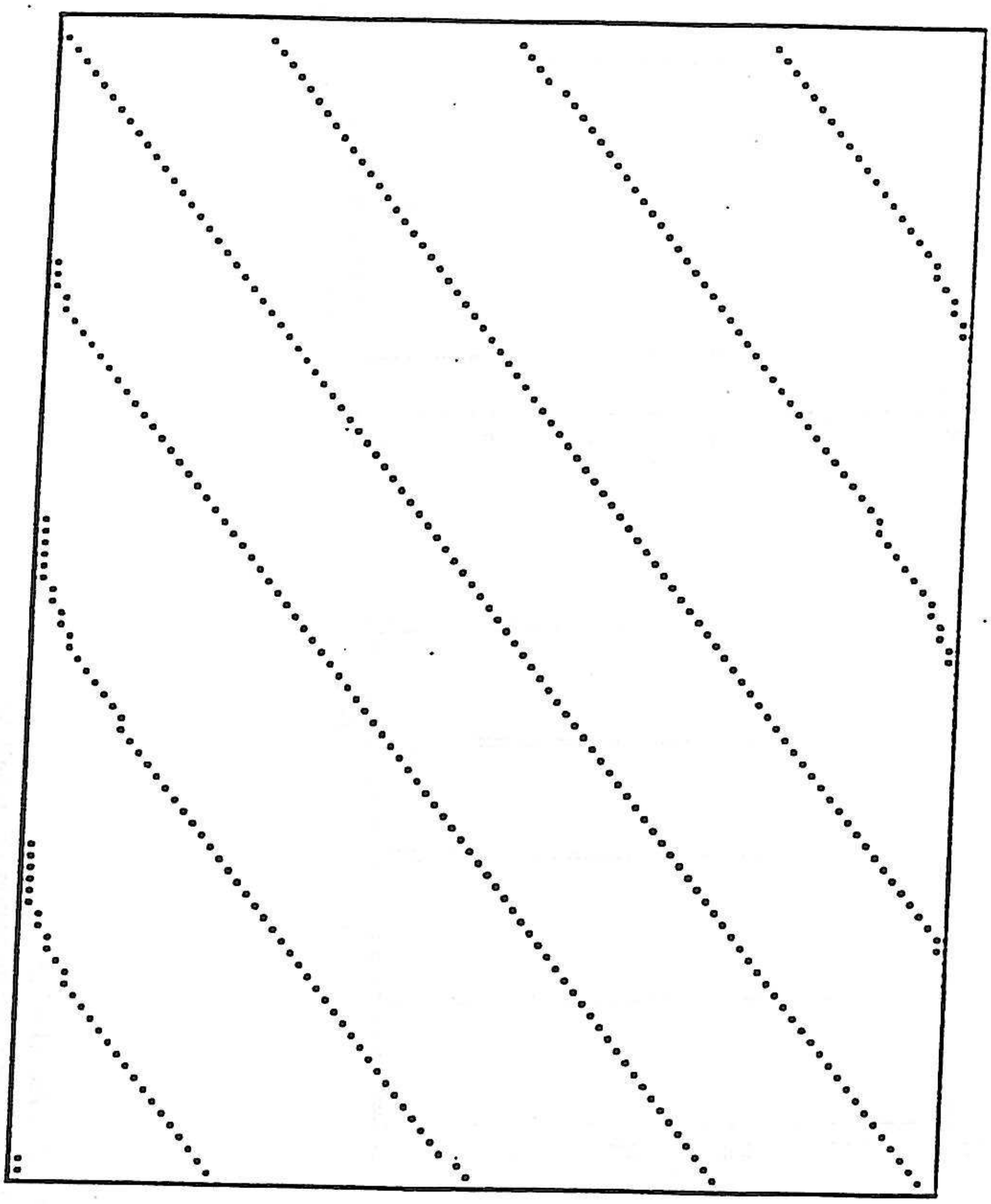
2. Concentration of component U in cell 50 in a developed stationary patterns as a function of amplitude of perturbation. Fig. 2b and Fig.2c are the magnifications of parts of Fig.2a.



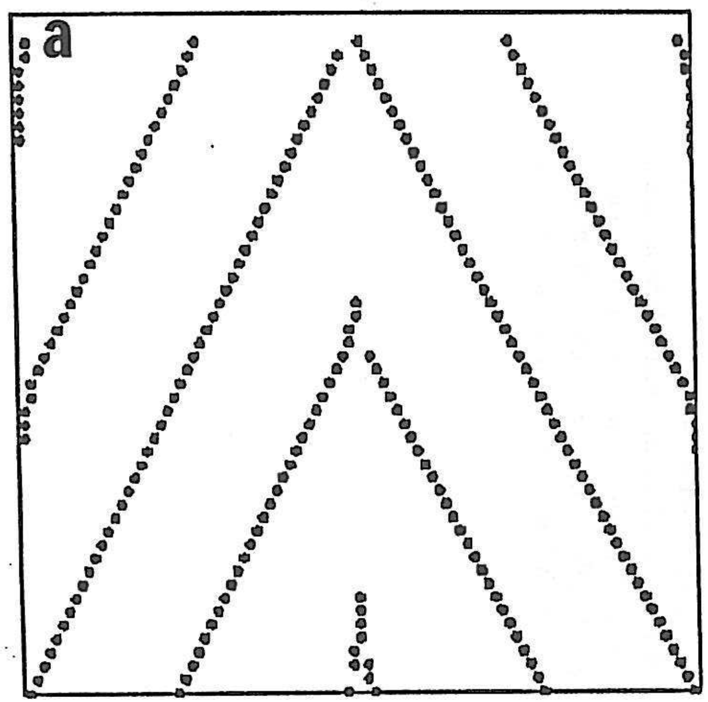
3. Stationary pattern developed after cells 50 and 51 were perturbed by a single perturbation. a) perturbation U=0.125, b) perturbation U=0.145, c) perturbation U=0.26. Developed patterns have four maxima.

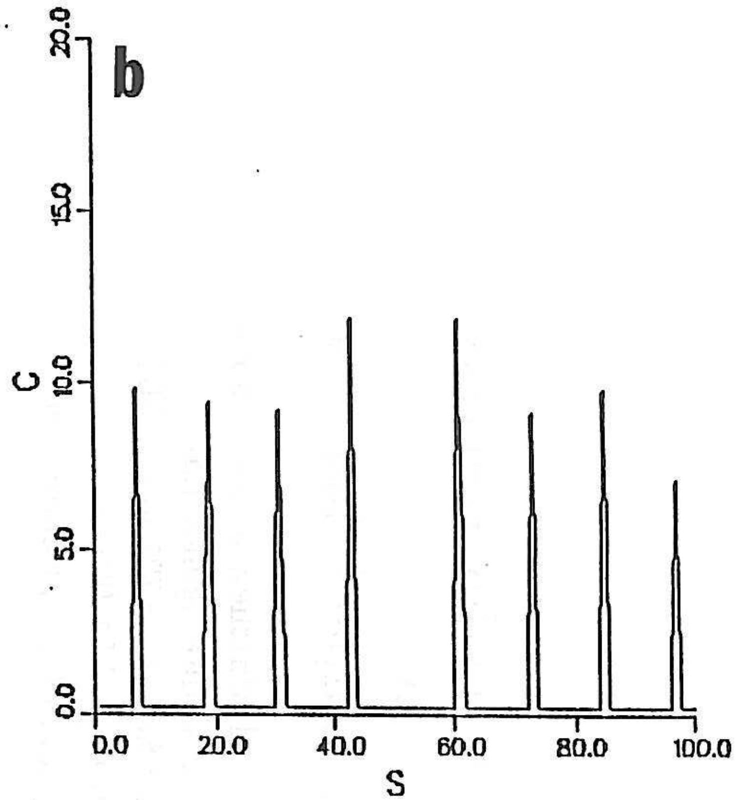


4. Memory effect. Amplitude of perturbations; U=5.0
   a) Stationary pattern developed after a single perturbation of a cell 50.
   b) Stationary pattern developed after a single perturbation of a cell 74,
   c) Stationary pattern developed after a single perturbation of a cell 89.



5. Representation of developed patterns as a function of the place of single perturbations. x-axis spatial coordinates (cells). Dots represent maxima on developed stationary patterns. y-axis positions of perturbations. The top first row represents the pattern developed after the cell 1 was perturbed, second row represents the pattern after the second cell was perturbed.





6. a) Representation of developed patterns as a function of a distance between two perturbation points. x-axis spatial coordinates, y-axis distance between two perturbation points (from top to bottom)
b) Example of pattern with eight maxima and two different wavelengths