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Research Paper

Mathematical investigation of two dimensional pattern formation

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Abstract

In this paper, one of the significant effects on two dimensional pattern formations of chemical reactions concerned with diffusion of species is investigated. Gray-Scott model is employed to study the effect of diffusion on reaction rate and distribution of the reactants. Nonlinear dimensionless partial differential equations of the problem are solved using explicit finite difference method. Contours of one agent are obtained for different parameter values and time dependencies of the patterns are investigated. Different time scales of the problem are also took into consideration.

Keywords: *Diffusion, finite difference method, Gray-Scott model, pattern formation, time scale.*

1. Introduction

Modeling natural systems and engineering problems plays significant role in controlling, manipulating and comprehension of these phenomena. Mathematicians and Engineers endeavor to offer a comprehensive model which can best illustrate properties of considered phenomena. Simplicity and accuracy are of outmost considerable factors to construct a model. For instance, biosensors as biological devices are used in many cases related to measurement, medical issues and food safety. In order to optimize and study features of biosensor, mathematical modeling is employed as a powerful method (Aris 1975). Amperometric biosensor at mixed enzyme kinetics in regard to diffusion limitation was also modeled and solved by Tonekaboni et al. (Tonekaboni *et al*. 2013). Another example in this case is drug delivery in which different models and theories such as erosion and chemical reaction-diffusion have been discussed and various mathematical models proposed during the last decades (Siepmann & Göpferich 2001). One of the interesting natural phenomena is animals' coats which can be related to pattern formation.

Pattern formation is among the important areas of research in developmental Biology. Spatial patterns cause emerging different patterns in the nature such as hair patterns and coat markings from a single cell. It has been figured out during the last decades that investigating a study of gene is not enough to understand the generation of the complicated spatiotemporal signaling lineup in early development. It is necessary to mathematically model the complex chemical and physical processes which play important role in different areas of developmental Biology. Turing model (Turing 1952) is among the most studied ones to model spatial pattern formation. His theory which is based on diffusion-driven instability, proposes that existence of diffusion of species in the system results in the non-uniform patterns in the system. For instance, consider U(x,t) and V(x,t) are the density functions of two species which interact or react. The following relations represent reaction-diffusion (1) and reaction equations (2) according to Turning's idea.

$$U_t = D_U \nabla^2 U + f(U,V)$$
$$V_t = D_V \nabla^2 V + g(U,V) \qquad (1)$$

$$U_t = f(U,V)$$
$$V_t = g(U,V) \qquad (2)$$

Although a constant solution of U(t,x), V(t,x) can be a stable solution of (2), it can be an unstable solution of (1). Thus the instability is induced by diffusion. In the other word there must be non-constant equilibrium solutions which have more complicated spatial structure.

In this case Murray (1993) suggests that a single mechanism could be responsible for generating all of the common patterns observed. This mechanism is based on a reaction-diffusion system of the morphogen pre-patterns, and the subsequent differentiation of the cells to produce melanin simply reflects the spatial patterns of morphogen concentration. Morphogen is defined as any of various chemicals in embryonic tissue that influence the movement and organization of cells during morphogenesis by forming a concentration gradient. Melanin is pigment that affects skin, eye, and hair color in humans and other mammals.

Because of the problems in identifying the morphogens, there was no experimental evidence about non-oscillatory steady patterns of Turing system until 1989 in which this phenomena was found in a real chemical reaction (Castets *et al.* 1990). Many of the experimental results can be exhibited by this model including spotted and stripped patterns (Maini 1997). Specifically, it has been presented that Turing system can be considered as an inductive mechanism for neural connections (Barrio & Zhang 1999, McLaughlin 2002, Leppnen *et al.* 2002). It is based on the concept of positional information and chemical signaling. Different models have been proposed during the last decades. Gray-

Scott model is among the models proposed to investigate the effects of diffusion on the pattern formation (Turing model). One of the well-known versions of this model was investigated by Pearson (1993) which is also used in this article.

The non-dimensional mathematical model presented by Pearson is used in this paper to investigate reaction-diffusion phenomena. Different patterns of the presented model are obtained numerically employing explicit finite difference approach and using Python 2.7.3 as a promising and fast programming language. Two dimensional contours are presented for aforementioned problem to clarify the behavior of the important variables in the model and effects of different parameter values on it. Two parameters are presented to show the dynamic behavior of the system and possibility of reaching to the steady state condition.

2. Mathematical modeling

Mathematical modeling of the considered problem, Gray-Scott model of reaction diffusion phenomena, is presented in this section. The purpose of the model is investigating different effects on reactions of chemical agents especially in biological contexts.

2.1. Gray-Scott model

In order to investigate the effects of diffusion of the two chemical agents during reaction procedure based on concentration gradients, the general Turing system can be written as follows:

$$\begin{aligned} \partial_t U &= D_U \nabla^2 U + f\left(U,V\right) \\ \partial_t V &= D_V \nabla^2 V + g\left(U,V\right) \end{aligned} \tag{3}$$

This general system of PDEs in the specific form of Gray-Scott model:

$$\begin{aligned} \frac{\partial U}{\partial t} &= D_U \nabla^2 U - UV^2 + F\left(1-U\right) \\ \frac{\partial V}{\partial t} &= D_V \nabla^2 V + UV^2 - \left(F+K\right)V \end{aligned} \tag{4}$$

Corresponds to the irreversible reaction of two species as follows:

$$\begin{aligned} &U + 2V \to 3V \\ &V \to P \end{aligned} \tag{5}$$

The considered two dimensional Gray-Scott models were investigated numerically and analytically by Pearson (1993). On the basis of the irreversibility of the reactions, P as the product of the procedure is an inert chemical. In the presented Gray-Scott model, F is the dimensionless feed rate which is based on the fact that, U is fed into the reaction. In addition, K is the dimensionless rate constant of the second reaction.

2.2. Numerical simulations

Explicit finite difference method (FDM) is employed to obtain the solution of the considered problem. The discretized form of the two PDEs of Gray-Scott model (3, 4) can be written as Eq. (6).

These equations are obtained using the second order central spatial derivative and forward first order temporal derivative. More information about the grid-size, time step and other information about the solution procedure are presented in the next section.

In the next section, the results of the considered Gray-Scott problem are presented which are obtained by employing the described numerical procedure to solve the nonlinear PDEs. Initial conditions used to obtain the results of the problems are described in the next section. As a usual boundary condition for biological and chemical problems, periodic boundary conditions are assumed to represent that this is a small region of a greater domain in the real system.

$$\begin{aligned} &\frac{U_{i,j}^{n+1} - U_{i,j}^{n}}{\Delta t} = \\ &D_U \left(\frac{U_{i+1,j}^{n} - 2U_{i,j}^{n} + U_{i-1,j}^{n}}{\Delta x^2} + \frac{U_{i,j+1}^{n} - 2U_{i,j}^{n} + U_{i,j-1}^{n}}{\Delta y^2} \right) \\ &- U_{i,j}^{n} \left(V_{i,j}^{n}\right)^2 + F\left(1 - U_{i,j}^{n}\right) \\ &\frac{V_{i,j}^{n+1} - V_{i,j}^{n}}{\Delta t} = \\ &D_V \left(\frac{V_{i+1,j}^{n} - 2V_{i,j}^{n} + V_{i-1,j}^{n}}{\Delta x^2} + \frac{V_{i,j+1}^{n} - 2V_{i,j}^{n} + V_{i,j-1}^{n}}{\Delta y^2} \right) \\ &+ U_{i,j}^{n} \left(V_{i,j}^{n}\right)^2 - \left(F + K\right) V_{i,j}^{n} \end{aligned} \tag{6}$$

3. Results and discussion

The results of Gray-Scott model of reaction-diffusion phenomena as an important problem in Chemistry, Physics and Biology are discussed in this section. The aforementioned nonlinear mathematical equations of the problem, solved using explicit FDM, have interesting behaviour for different parameter values presented in this section. As a time dependent problem, dynamic behaviour of the system and possibility of existence of approximate steady state solution are investigated for different parameter values of the problem.

In order to obtain the results of Gray-Scott model, the 20×20 mesh point region in the middle of the considered domain system initially perturbed to U=1/2; V=1/4 (Fig. 1). The domain also consists of 256×256 grid points where total system size is assumed to be 2.5×2.5. In addition, $D_U=2\times10^{-5}$ and $D_V=10^{-5}$ are considered as values of diffusion coefficients for all the obtained patterns. Furthermore, the values of F and K are chosen corresponding to the values presented by Pearson (1993) which are shown in Table 1. In Fig. 1 and all patterns of Fig. 2, concentrations of U are shown by red, blue and yellow corresponding to U=1; U≈0.5 and intermediate concentrations, respectively. The parameter values presented in Table 1 are leading to different patterns of the Gray-Scott model shown in Fig. 2. These contours are obtained at t=120,000 and similar to the results of Pearson. One of the important parameters in this problem modeling reaction-diffusion phenomena is propagation velocity of the species. It is obtained in the simulations that after around 20,000 time steps the perturbed concentration in the middle of the domain reaches to the boundaries in all cases. Therefore, the propagation velocity can be considered in the order of 10^{-5} space units per time unit.

The different patterns presented in Fig. 2 corresponding to parameter values of Table 1 can be categorized based on two points of view. The first one is about existence of spots or strips in the patterns and the other one is about dynamic behavior of patterns and possibility of existence of steady state solution at large time scale. In order to clearly show the dynamic behavior of each patterns, another parameter, $AL=\sum_{(i,j)}(|\nabla^2 V|+|\nabla^2 U|)$, is defined and its variations versus time are presented in Fig. 3 for the patterns depicted in Fig. 2.

Table 1: Parameter values of different patterns used for Gray-Scott model

Pattern	α	ϵ	γ	δ	λ	κ
F	0.02	0.02	0.024	0.033	0.03	0.05
K	0.05	0.056	0.056	0.056	0.064	0.064

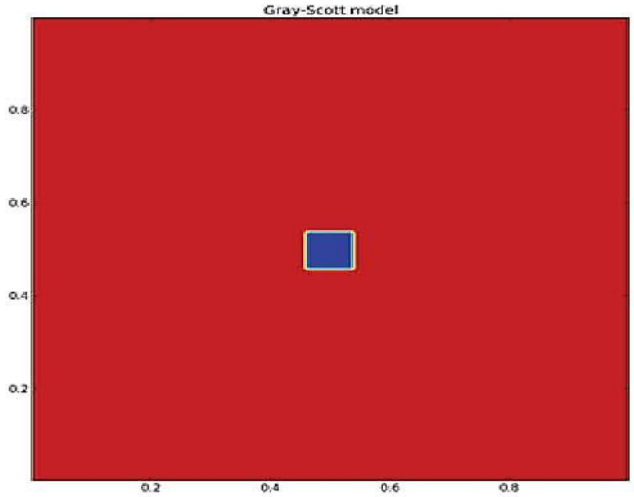

Fig. 1: Initial condition of all patterns considered for gray-Scott problem.

It is clearly illustrated in Fig. 2 that patterns ϵ, δ and λ are more like spotted patterns and the other ones are more like striped patterns. In the spotted patterns, there is a background network in which regions of same concentration connect together and some small spotted ones specify the island like regions throughout the domain. These spots in some cases correspond to low concentrations (Fig. 2 (e)) and in some other cases are related to higher concentrations (Fig. 2 (d)). In pattern λ, the spots occur only in the regions that the uniform steady state is the red one. Because of requirement of gradient for existence of spots, there should be a maximum size. Otherwise, the gradient free blue regions exist in the domain and decay to the steady state. In some of the patterns such as δ (Fig. 2 (d)) regular patterns (regular hexagonal patterns) can be formed. Nevertheless, there are some other ones consisting irregular spotted patterns such as ϵ (Fig. 2 (b)). Regularity of patterns sometimes can be important to design chemical reactions or investigate biological reactions. In order to better control a system, regular behavior and pattern are more suitable.

On the other hand, the striped patterns do not let any completely connected background be formed (Fig. 2 (f)). In this kind of pattern, stripes cause separation of different parts of background. In some cases such as Fig. 2 (a) corresponding to pattern α full spirals cannot be formed.

The dynamic behavior of different obtained patterns is illustrated in Fig. 3.

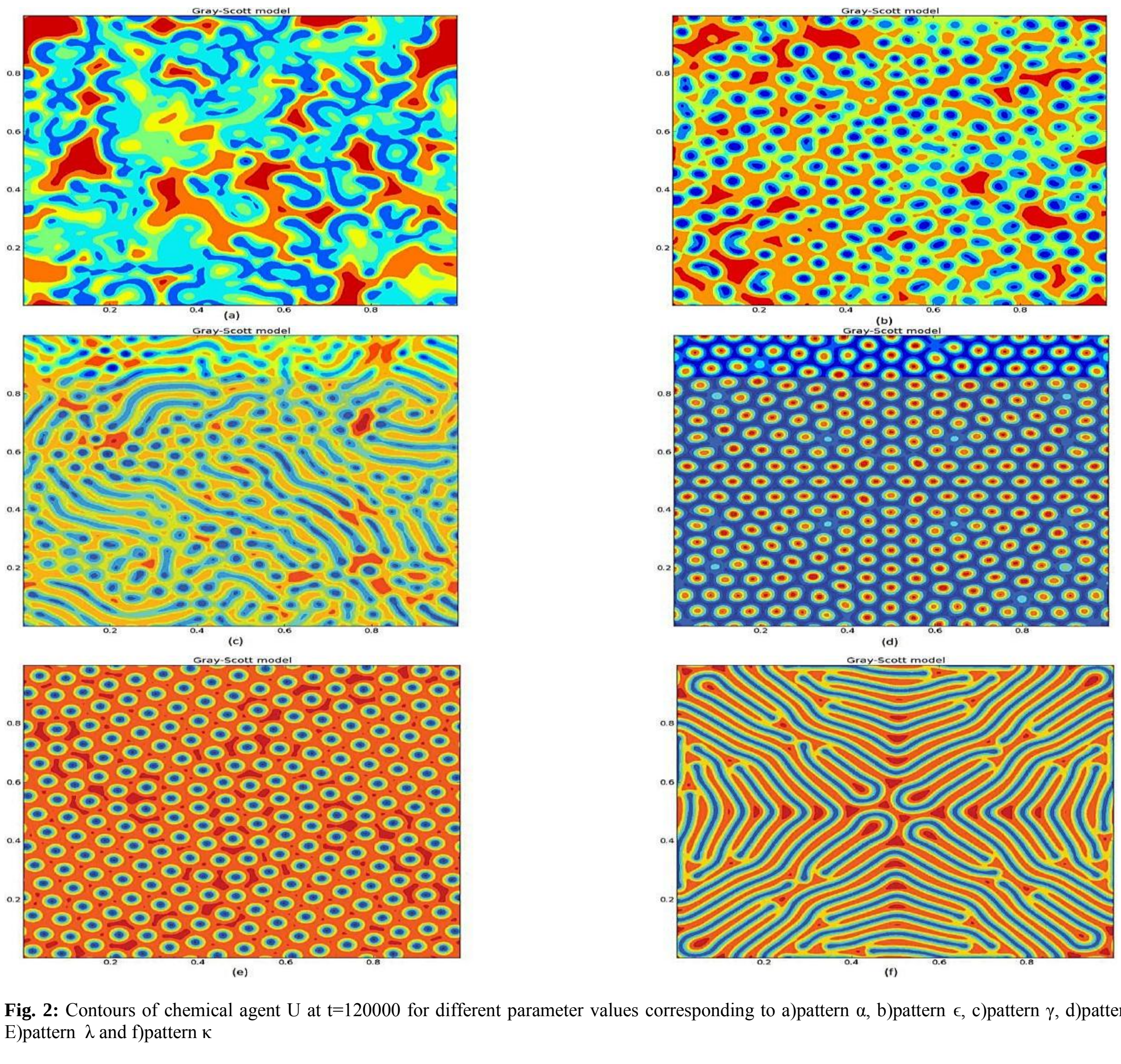

Fig. 2: Contours of chemical agent U at t=120000 for different parameter values corresponding to a)pattern α, b)pattern ϵ, c)pattern γ, d)pattern δ. E)pattern λ and f)pattern κ

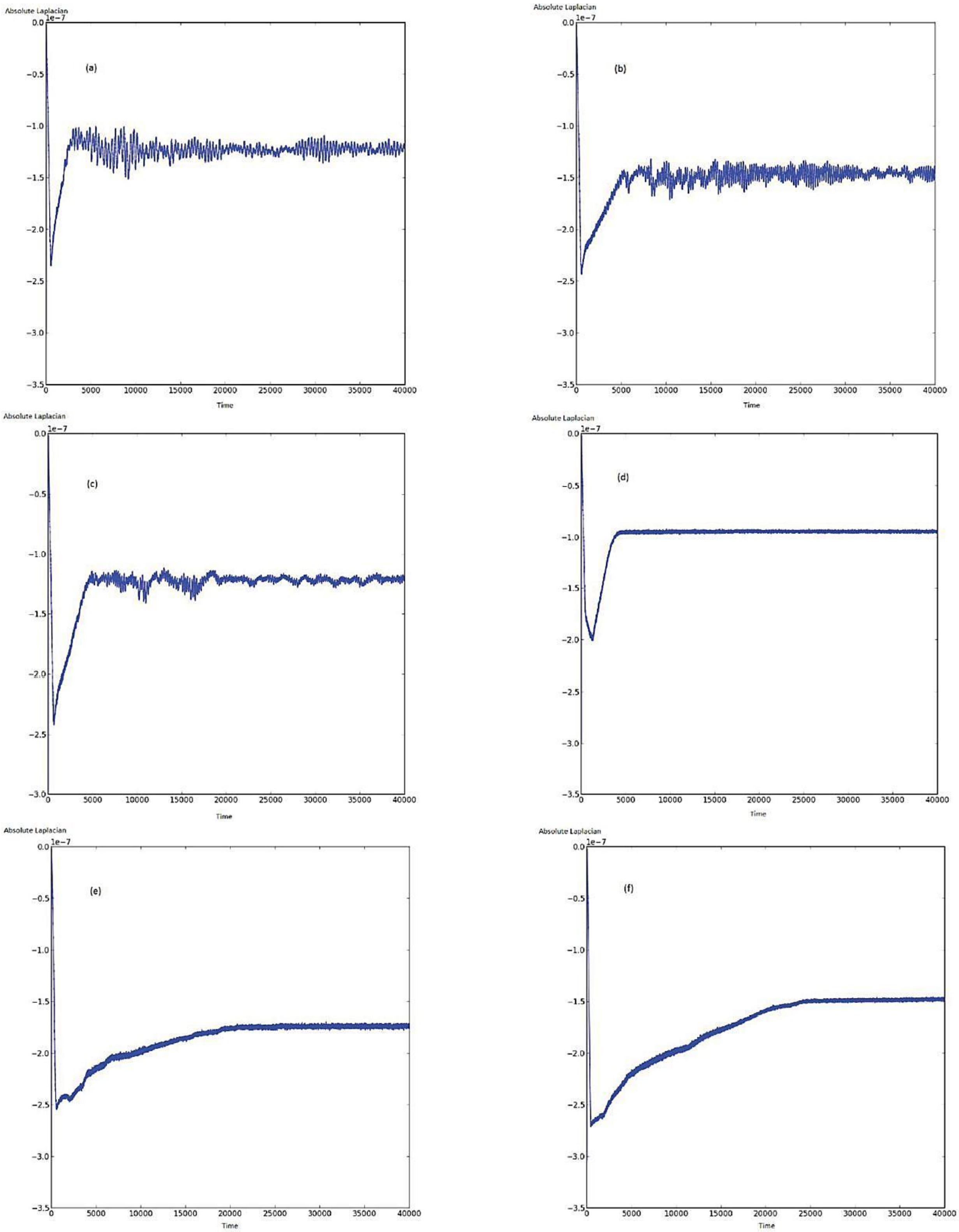

Fig. 3: Variation of $\boldsymbol{AL}$ versus time a)pattern $\boldsymbol{\alpha}$, b)pattern $\boldsymbol{\epsilon}$, c)pattern $\boldsymbol{\gamma}$, d)pattern $\boldsymbol{\delta}$. E)pattern $\boldsymbol{\lambda}$ and f)pattern $\boldsymbol{\kappa}$

As a result of the considered initial condition, there is fast change in beginning of the diagrams of Fig. 3. It is shown that oscillatory behavior or steady state condition starts in the range of t=5,000 and t=20,000 corresponding to the time stages the initial perturbed concentration reaches the boundaries of the domains. Therefore, as it has been mentioned before, the propagation velocity for all patterns is approximately in the order of 10^{-4}.

It is shown in this figure that patterns δ, λ and κ reach approximately steady state conditions. The time stages in which each of these patterns reaches their approximate steady state conditions are different. Pattern δ converges to its steady state so faster than the others. Patterns λ and κ approximately behave in the same way, but λ reaches to its steady state faster than κ.

It should be noted that all of these patterns have small defects oscillating with high frequency. It is an interesting phenomenon that regular and symmetric patterns (Fig. 2 (d), (e) and (f)) reach to their steady state concentration distribution in the domain. In the other transient patterns, variations of the considered parameter by time are not like regular oscillatory behavior and their frequency and amplitude change versus time.

4. Conclusion

The mathematical modelling of the effects of diffusion and phase transition on two dimensional chemical reactions are investigated. Nonlinear partial differential equations of the problem are presented in the dimensionless form to be able to investigate the problems generally.

Effects of diffusion on reaction of the chemical agent known as reaction-diffusion phenomena are modelled using Gray-Scott formulation. The presented nonlinear PDEs are solved employing explicit finite difference method and using suitable time step and grid size. Boundary conditions of problem are considered to be periodic to represent a region of a bigger domain.

In order to obtain contours of Gray-Scott model, values of parameters F and K are chosen from Pearson (1993). Moreover, results are similar to Pearson. Contours of different patterns exhibit various shapes generally classified into spotted patterns (ε, δ, λ) and striped patterns (α, γ, κ) according to their specified parameter values. The other important factor which is dynamic behavior of patterns was studied and steady and transient states were obtained. All patterns are in the same order (10^{-4}) for their propagation velocity. Eventually, steady states conditions of patterns according to the boundary conditions and different determined parameters are investigated.

Contours of U as one of the species in the Gray-Scott model are presented for different parameter values at t=20,000. Time dependency of the patterns is also investigated using variation of a new defined parameter as sum of absolute Laplacians of the species throughout the domain. It is shown that three of the illustrated patterns are time-dependent and the other ones reach to approximate steady state after a while.

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