A Numerical Study of One-Dimensional Replicating Patterns in Reaction-Diffusion Systems with Non-Linear Diffusion Coefficients

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ABSTRACT

A numerical study of the dynamics of pattern evolution in reaction-diffusion systems is performed, although limited to one spatial dimension. The diffusion coefficients are non-linear, based on powers of the scalar variables. The system keeps the dynamics of previous studies in the literature, but the presence of non-linear diffusion generates a field of strong non-linear interactions due to the presence of receding travelling waves. This field is limited by the plane of symmetry of the space domain and the last born outgoing travelling wave. These effects are discussed.

INTRODUCTION

Non-linear reaction-diffusion (R-D) equations play an important role in many subjects in the science and technology. The ever-growing interest in the analysis and in obtaining the solution for particular problems may be easily verified in the impressive growth of relevant literature. One of the most interesting peculiarities present in the solution of R-D equations is the time evolution of patterns of reactant concentrations.

In the last years, some new characteristics of pattern evolution in two-dimensional R-D systems have been observed, notably by Pearson [1]. Dawson et al. [2] studied some implications of R-D equations in biological systems. Also recently, Reynolds et al. [3] performed an analytical analysis of the evolution of patterns in one-dimensional (1-D) problems. Lee et al. [4,5] considered the formation of patterns by interaction of chemical fronts. The work by Hagberg [6] and its sequel and by Hagberg and Meron [7] elucidated many aspects of front dynamics in R-D systems. Recently Barach [8] studied the evolution of the solution of the model equations of [1]. These systems have also been used as mimic models of biological systems [9]. Much has been written in all these cases, even very recently and we are not attempting here a detailed review of results. This brief list is intended to cite only a few, recent papers dealing with the subject under consideration.

The equations considered here are of the form:

\[
\frac{\partial u}{\partial t} = D \cdot \frac{\partial}{\partial x} \left[ u^m \frac{\partial u}{\partial x} \right] - u \cdot v^2 + F \cdot (1 - u)
\]

\[
\frac{\partial v}{\partial t} = d \cdot \frac{\partial}{\partial x} \left[ v^m \frac{\partial v}{\partial x} \right] + u \cdot v^2 - G \cdot v
\]

Equations (1) are of the same form as those in [2], with \(F=0.02\), \(G=0.079\), \(D=1\) and \(d=0.01\), but now include a non-linear diffusion (NLD) coefficient, i.e. \(m \neq 0\).
Consideration of non coupling in equations (1) (and \( m=3, F=G=0 \)) leads to the case of viscous, gravity driven flows, such as the spreading of wetting liquids in plane surfaces. The most recent results of the authors on non-linear diffusion come from this field [10].

As mentioned before, we will consider in some detail the numerical solution of equation (1) with NLD coefficients. The main interest of this analysis comes from the possibility of taking into account the effect of R-D terms in travelling wave (TW) solutions to said equations. It is interesting to point out that the non-linear diffusion coefficient implies the existence of an effective advective term, measured by \( \mu m^{-1} \frac{\partial u}{\partial x} \) times the physical diffusion coefficient. The advective behavior of the solution of equations (1) comes from this term and, in the case of pure non-linear diffusion leads to TW solutions. This effect is not present, of course, when \( m=0 \).

The analysis will be restricted to 1-D because of the limitations in the computer resources available. This limitation may put a limit in the interest of the patterns to be observed. However, despite this assumption, the essential aspects of the dynamics will be kept.

**ANALYSIS**

Equations (1) were solved by means of explicit, forward-time, space-centred finite-differences scheme, in an integration domain defined by: \( x \geq 0, t > 0 \). The time interval was \( T \) and will be specified in what follows. To be consistent with the results originally quoted in references [2,3], a uniform spacing of the calculation points was adopted, namely: \( \Delta x = 0.5 \). The number of nodes varied according to:

- the type of boundary conditions (BCs),
- the symmetry of the problem, and
- the number of time steps, \( N_T \), to span the time interval \( T \).

The number of nodes, \( N_x \), ranged between 200 and 1000. The changes in the number of nodes come from the need of avoiding the effect of the finite size of the spatial integration domain and from considering different BCs. The time step was fixed at \( \Delta t =0.01 \), further reduction was not necessary to improve the results.

In the 1-D cases studied, the sequence of steps for the calculations was:

- at \( t=0 \) a perturbation for \( u \) and \( v \) was introduced in the otherwise uniform field \( u=v=0 \). These perturbations were in the form of a rapidly spatially decaying exponential, spanning 1/20th of the spatial domain. The maximum values were \( u=1, v=0.25 \).
- Usually, integration was performed up to \( T=4000 \).
- Different plots were performed. However, the most interesting were the ones corresponding to the activator \( v \), conveniently shifted in the ordinates to show the evolution of the fronts as time elapsed. This type of plot is also found in [3]. The number of time steps between lines was \( N_T = 4000 \).

The evolution of the dynamics of \( u, v \) in the case \( m=0 \), has been described in terms of an interesting analogy in [3]. It was also shown in [2]: soon after the initial perturbation sets up, a branch in the activator distribution appears. It generates two peaks that begin to separate. After they reach a critical distance, a new branch shows up. It eventually grows and leads to the appearance of two differentiated peaks, which again begin to separate. The process may repeat, leading to a stationary distribution of peaks and valleys (limited by the finite size of the spatial, periodic domain). This stationary state cannot be attained with NLD coefficients.
RESULTS

Figure 1 shows the results obtained for the case similar to the one in [3], namely:

- m=0, D=1, d=0.05, Δt =0.01, Δx = 0.5, Nx=201, T=4000, periodic BCs.

This will be considered as the reference data set. It is worth mentioning that the exponential was adopted as the initial perturbation after having found that a step like variation made the replication pattern onset depending on the step span. It became evident when plane symmetry at the left boundary (and no flux at the right one) was considered. Consequently, after the identity of the results obtained with the periodic BCs and plane symmetry BCs was carefully checked, the exponential was adopted for all the calculations. Figure 2 shows a detail of the steady-state distribution of u and v. The periodicity of the solution may be easily verified.

Considering linear advection in this case only translates the whole field, without dramatic changes in the pattern configuration. This conclusion is limited to small cell Peclet number \( P = C \Delta x/D \), where \( C \) is the advection velocity (d must be considered for v).

In what follows the effect of different values for m will be addressed. A few results will be shown here. The analysis of the complete set of results will be the matter of another paper. The first notable difference in using \( m \neq 0 \) is that the replication pattern arises, as expected, in a TW context. Figures 3 and 4 show how the pattern looks like for the following data set:

- m=3, D=1, d=1, Δt =0.01, Δx = 0.5, Nx=201, T=800, periodic BCs.

In this case the time interval was limited to T=800 because periodic BC’s now impose dynamic interaction of advancing and receding fronts. From this data it must be observed that d=1 means that the acting diffusivity for v will be \( v^2 \), what in turn means a varying coefficient of the order of the original one. The same reasoning applies to u. The first property observed is the different pattern configuration and the different velocity of front propagation. The interaction is different too. The receding fronts interact very strongly near the plane of symmetry. They begin to replicate limited by the main peaks travelling to the sides. In the overall, it may be observed that the critical distance for branching is now smaller in the central zone. Furthermore, after the original branch, peaks travelling to the sides do not seem to branch anymore.

Figure 5 shows (considering plane symmetry and Nx=201) the early development of the case in figure 3 and 4. To allow further development of the pattern the following case was considered:

- m=3, D=1, d=1, Δt =0.01, Δx = 0.5, Nx=1001, T=4000, BCs with plane symmetry

Figure 6 shows the pattern evolution, while Figure 7 shows a detail of the spatial distribution for \( T= 4000 \), i.e. \( NT = 400000 \).

Cases have been also considered for \( m = 4 \) and \( 5 \). No symmetry has been imposed and the one corresponding to \( m = 5 \) shows branching in the far side running peaks. This implies that the lack of appearance of further branching for \( m=3, 4 \) may be due to values of \( v^2 \) not low enough with respect to \( u^3 \). This fact was expected, but it is unfortunate, because no simple scaling seems possible to make calculations comparable.

It is worth mentioning that, due to symmetry and the TW behavior of the pattern, a continuous source of information exists at the \( x = 0 \). The fronts interacting in this zone bifurcate and interact with each other in a spatial domain restricted by the trailing edge of outgoing fronts. This interaction and the continuous supply of energy from the source term assure the indefinite duration of this process.
CONCLUSIONS

The results obtained confirmed the presumptions concerning existence of a travelling wave pattern of replicating structures in reaction-diffusion systems. This is interesting because allows the propagation of information at a finite velocity, despite the diffusion-like characteristics of the system. In addition, due to the presence of receding fronts, a pattern of continuous generation of new fronts exists. This is a source of new information, emerging from the origin. Further research will consider additional types of symmetries.

REFERENCES

Figure 1. Simulation of the pattern of the 1-D replicating R-D system of [3].
m=0, D=1, d=0.05, Δx=0.5, Δt=0.01, T=4000, periodic BC’s
Vertical axis: 100 v(x) + t, horizontal axis proportional to x.
Figure 2. Detailed view of the results of Figure 1, $u, v$ spatial distribution for $t=4000$
**Figure 3.** Early evolution of NLD-TW replicating pattern

$m=0$, $D=1$, $d=0.05$, $\Delta x=0.5$, $\Delta t=0.01$, $T=800$, periodic BC's

Vertical axis: $100 \, v(x) + t$, horizontal axis proportional $t$

**Figure 4.** Early evolution of NLD-TW replicating pattern

Spatial distribution of $u,v$. Time: $t=800$
Figure 5. Early evolution of the NLD-TW replicating pattern. 
m=3, Δx=0.5, Δt=0.01, Nx=201, T=800, symmetric BC’s
Vertical axis: 100 v(x) + t, horizontal axis proportional to x.
Figure 6. Time evolution of NLD-TW replicating pattern
m=0, Δx=0.5, Δt=0.01, Nx=1001, T=4000, plane symm. BC's
Vertical axis: 100 v(x) + t, horizontal axis proportional t
Figure 7. Detailed view of the results of Figure 6
u, v spatial distribution for t=4000