Robustness of spiral waves in two-dimensional reactive–diffusive media

J.I. Ramos

Room I-320-D, E.T.S. Ingenieros Industriales, Universidad de Málaga, 29013 Málaga, Spain

Abstract

The effects of the reaction terms, diffusion coefficients and size of the computational domain on the dynamics of the two-equation Oregonator model in two-dimensional reactive–diffusive media is studied numerically, and it is shown that spiral waves are robust under truncation or expansion of the computational domain. It is also shown that large diffusion coefficients for the inhibitor may result on either annihilation of the wave or unbounded growth, whereas large diffusion coefficients for the activator concentration may result in unbounded decay of both the activator's and inhibitor's concentrations. Small diffusion coefficients of the inhibitor may result in stationary tongue-like shapes, whereas small diffusion coefficients of the activator may result in narrow ring shapes where the activator's concentration is high. A decrease in the parameter which controls the stiffness of the activator's reaction rate is found to result in unbounded growth of the activator's concentration, whereas an increase in the parameter that couples the activator and inhibitor is found to result in either annihilation of the spiral wave or unbounded growth of the concentrations of both the activator and the inhibitor.

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Keywords: Spiral waves; Oregonator model; Domain truncation; Shadow systems; Sensitivity

1. Introduction

Spiral waves have been observed in many chemical and biological systems [1–4] as well as in numerical solutions of the reaction–diffusion equations that model such systems. One particularly interesting property of spiral waves is
their robustness with respect to the domain boundaries. In addition, spiral waves can become unstable in various ways, e.g., they can experience core and far-field instabilities, begin to meander and drift, break up, etc. [5,6,8]. For example, Wellner et al. [6] considered the drift of stable, meandering spiral waves in a singly diffusive FitzHugh–Nagumo medium caused by a weak time-independent gradient or convection in the fast-variable equation, showed by means of perturbation methods the equivalence between gradient and convective perturbations, and proposed a semiempirical solution to the drift of spiral waves that depends on the period of rotation and the value of the fast variable at the center of the spiral wave.

Biktashev and Holden [7] and Zhang and Holden [5] have explained the hypermeander of spiral waves as a chaotic attractor that leads to a motion of the spiral wave tip analogous to that of a Brownian particle. On the other hand, Biktashev et al. [8,9] considered an excitable medium in two dimensions with a cubic nonlinearity given by the FitzHugh–Nagumo system and a shear characterized by a velocity field in the x-direction which is either a linear or a sinusoidal function of the y-coordinate, and showed that the shear can distort and then destroy spiral waves. Such breaks were found to result in a chain reaction of spiral wave births and deaths. The velocity fields employed by Biktashev et al. [8] are one-directional and solenoidal, but not irrotational, and they do not satisfy the no-penetration condition at the boundaries of the domain; in fact, these authors used periodicity conditions for the sinusoidal velocity field. Elkin et al. [10] have studied numerically the movement of excitation wave breaks, while Biktashev and Holden [11] analyzed the resonant drift of autowave vortices in two-dimensional reactive–diffusive and the effects of boundaries and inhomogeneities. Other numerical studies have shown that the propagation of spiral waves in two-dimensional excitable media depends on the applied velocity field, its rotation and its straining, as well as the boundary conditions [12–14]. Most of the numerical studies on spiral wave propagation performed to-date have considered homogeneous Neumann boundary conditions.

In order to both clarify and understand the stability of spiral waves, the persistence of spirals and the behavior of their spectral properties under domain truncation, approaches that use the spatial dynamics of elliptic steady-state equations have been proposed [15]. Unfortunately, these analytical studies have considered only steady state conditions, and have not taken into consideration the effects of the boundary conditions on the stability and persistence of spiral waves. One objective of the numerical study presented here is to assess the influence of the size of the two-dimensional excitable media on the stability, persistence and/or break-up of spiral waves in two-dimensional excitable media.

A shadow system appears as a limit of a reaction–diffusion system in which some components have infinite diffusivity. It is known that, unlike scalar re-
action–diffusion equations, the shadow system may exhibit various interesting phenomena such as spontaneous spatio-temporal pattern formation. On the other hand, it is also known that, in autonomous shadow systems on a compact interval, any nonconstant nonmonotone stationary solution is necessarily unstable. Although the dynamics of shadow systems in a general setting can be analyzed by applying the theory of Floquet bundles, it has been found that any stable bounded (not necessarily stationary) solution is either asymptotically homogeneous or eventually monotone in space [16]. The second objective of the numerical study presented here is to report some results on shadow systems of the two-equation Oregonator model when the diffusivity of either the activator or the inhibitor is very large, and to assess the effects of the parameters that influence the reaction rates on the propagation of spiral waves in two-dimensional reactive–diffusive media.

2. Governing equations

The numerical study presented here is based on the Belousov–Zhabotinsky (BZ) reaction which is often modelled by the Oregonator equations [1,17] and may be written as

\[
\frac{\partial u}{\partial t} = \nabla \cdot (D_u \nabla u) + F_u, \tag{1}
\]

\[
\frac{\partial v}{\partial t} = \nabla \cdot (D_v \nabla v) + F_v, \tag{2}
\]

where \( t \) is time, \( u \) and \( v \) denote the concentrations of the activator and the inhibitor, respectively, \( D_u \) and \( D_v \) are the diffusivity tensors for \( u \) and \( v \), respectively, and the source terms in Eqs. (1) and (2) can be written as

\[
F_u = \frac{1}{\epsilon} \left( u - u^2 - f v \frac{u - q}{u + q} \right), \quad F_v = u - v, \tag{3}
\]

where, unless stated otherwise, \( \epsilon = 0.01 \), \( f = 1.4 \) and \( q = 0.002 \), and are the same as those employed in the BZ model.

In this paper, it is assumed that \( D_u = d_u I \) and \( D_v = d_v I \) where \( I \) is the unit tensor of second rank, and it is known that, for \( d_u = 1 \) and \( d_v = 0.6 \), the Oregonator model has spiral wave solutions if homogeneous Neumann boundary conditions are applied at the boundaries.

Eqs. (1) and (2) were solved in the spatial domain \( \Omega = [-L_x, L_x] \times [-L_y, L_y] \) with, unless stated otherwise, \( L_x = L_y = 7.5 \), subject to homogeneous Neumann boundary conditions on all the boundaries.

The initial conditions in \( \Omega \) for Eqs. (1) and (2) are

\[
u = 0 \quad \text{for} \quad 0 < \theta < 0.5; \quad u = q(f + 1)/(f - 1) \quad \text{elsewhere,} \tag{4} \]
\[ v = q \frac{f + 1}{f - 1} + \frac{\theta}{8\pi f}, \]  
\[ \text{(5)} \]

where \( \theta \) is the angle with respect to the origin of coordinates measured counter-clockwise from the positive \( x \)-axis. This initial condition results in the formation of a spiral wave which rotates counter-clockwise if homogeneous Neumann boundary conditions are applied on all the boundaries.

Eqs. (1) and (2) were solved numerically by means of an implicit, time-linearized, second-order accurate (in both space and time) finite difference method [18]. This method factorizes the elliptic equations that result upon discretization of time at each time level, into two one-dimensional boundary value problems and employs an iterative technique to account for the approximate factorization errors. Computations were performed on a \( 1000 \times 1000 \) point equally-spaced mesh and a time step of \( 10^{-4} \). Computations were also performed with equally-spaced meshes of \( 200 \times 200 \) and \( 500 \times 500 \) points and different time steps in order to ensure that the results were independent of both the number of grid points and the time step. In the next section, some sample results obtained with \( 1000 \times 1000 \) point equally-spaced meshes and a time step equal to \( 10^{-4} \) are presented; however, only \( 102 \times 102 \) points are illustrated in the graphs.

3. Presentation of results

In this section, some sample results illustrating the effects of the lengths \( L_x \) and \( L_y \) of the computational domain, and \( d_u, d_v, f, q \) and \( \epsilon \) on the spiral wave propagation are presented. Before such an illustration is undertaken and in order to provide a firm justification of the results reported in this section, it is convenient to emphasize that the parameters that control the reaction rate are \( f, q \) and \( \epsilon \) (cf. Eq. (3)). We shall refer to \( \epsilon \) as the stiffness parameter, because a decrease in \( \epsilon \) provides a dramatic increase (decrease) of \( F_u \) (cf. Eq. (3)) if the term within parentheses in Eq. (3) is positive (negative). The parameter \( f \) is here referred to as the coupling parameter because if \( f \neq 0 \), \( u \) and \( v \) are coupled, whereas if \( f = 0 \), the activator’s concentration is uncoupled from the inhibitor’s concentration. Since, for the parameters mentioned in the previous section \( u < 1 \), the first two terms of \( \epsilon F_u \) add to a positive number smaller than unity and, therefore, the third term of \( F_u \) could become larger than the first two terms if \( f \) is sufficiently large.

The third parameter in Eq. (3) is \( q \) and, for \( u \geq 0 \), the third term in \( F_u \) changes sign whenever \( u = q \); therefore, this term changes sign when \( u \) becomes of the same magnitude as \( q \). Moreover, if the third term in \( F_u \) becomes negative where \( u \) is small and positive, \( F_u \) can be a large number if \( \epsilon \) is small, and this positive large number may result in large values of \( u \).
For $f = 1.4$, $e = 0.01$ and $q = 0.002$, a counter-clockwise spiral wave was observed [17] and the separation between two successive peaks of $u$ was found to be 1.61. The results presented in Fig. 1 indicate that, for $f = 1.4$, $e = 0.1$ and $q = 0.002$, a rounded and smooth spiral wave is obtained. This wave is thicker and more rounded than that corresponding to $f = 1.4$, $e = 0.01$ and $q = 0.002$. The results presented in Table 1 also indicate that the separation between and the width of the pulses in $u$ and the maximum value of $v$ at $(x, y) = (20\delta, 20\delta)$ where $\delta = 15/101$, increase, whereas the maximum value of $u$ at the same location decreases as $e$ is increased from 0.01 to 0.1. For $f = 1.4$ and $q = 0.002$, it has been observed that $\epsilon > 0.1$ results in almost annihilation or extinction of the spiral wave because the reaction terms for the activator decrease substantially as $\epsilon$ is increased.

For $f = 1.4$, $e = 0.001$ and $q = 0.002$, it has been observed that $u(20\delta, 20\delta, t)$ and $u(25\delta, 20\delta, t)$ grow almost linearly with time and their values at $t = 100$ exceed 950 and 625, respectively, whereas $v(20\delta, 20\delta, t)$ and $v(25\delta, 20\delta, t)$

Fig. 1. Concentration of the activator $u$ at (from left to right, from top to bottom) $t = 102.4$, 102.6, 102.8, 103, 103.2, 103.4, 103.6, 103.8 and 104 ($d_u = 1$, $d_v = 0.6$, $f = 1.4$, $q = 0.002$, $\epsilon = 0.1$, $L_x = L_y = 7.5$).
decrease almost linearly with time and their values at \( t = 100 \) are smaller than \(-2.5 \times 10^5\) and \(-6.5 \times 10^5\), respectively. For \( f = 1.4, \epsilon = 0.00001 \) and \( q = 0.002 \), it has been found that \( u(20\delta, 20\delta, t) \) and \( u(25\delta, 20\delta, t) \) decrease almost linearly with time and their values at \( t = 100 \) are smaller than \(-3.95 \times 10^5\), whereas \( v(20\delta, 20\delta, t) \) and \( v(25\delta, 20\delta, t) \) decrease almost linearly with time and their values at \( t = 100 \) are smaller than \(-1.95 \times 10^5\). The results just described indicate that Eqs. (1) and (2) are highly sensitive to \( \epsilon \) and their stiffness increases as \( \epsilon \) is decreased. Since the concentrations of both the activator and the inhibitor must be positive or nil, it must be stated that the two-equation Oregonator model is inappropriate for \( f = 1.4 \) and \( q = 0.002 \), and \( \epsilon < 0.01 \).

For \( q = 0.002 \) and \( \epsilon = 0.01 \), the results presented in Table 1 indicate that a spiral wave is observed for \( f = 1.4 \), whereas the activator’s concentration becomes uniform for \( f = 14 \), i.e., the spiral wave is annihilated for large values of \( f \). On the other hand, for \( f = 0.14, q = 0.002 \) and \( \epsilon = 0.01 \), it has been found that \( u(20\delta, 20\delta, t) \) and \( u(25\delta, 20\delta, t) \), and \( v(20\delta, 20\delta, t) \) and \( v(25\delta, 20\delta, t) \) decrease almost linearly with time and their values at \( t = 100 \) are smaller than \(-3.95 \times 10^8\) and \(-1.95 \times 10^8\), respectively.

Table 1 also shows that, for fixed values of \( f = 1.4 \) and \( \epsilon = 0.01 \), the separation between successive pulses and the maximum value of \( u \) at \((x,y) = (20\delta, 20\delta)\) decrease, whereas the width of the pulses and the largest value of \( v \) at the same location increase as \( q \) is increased from 0.002 to 0.02. However, for \( f = 1.4, q = 0.0002 \) and \( \epsilon = 0.01 \), similar results to those corresponding to \( f = 0.14, q = 0.002 \) and \( \epsilon = 0.01 \) were found.

For \( f = 1.4, q = 0.02 \) and \( \epsilon = 0.01 \), the concentration of the activator does not show a spiral wave, but an almost skew-symmetric shape with respect to one of the diagonals of the computational domain as indicated in Fig. 2, where it is observed that a curved high concentration front propagates from the upper right corner of the domain and reaches the left boundary creating a high concentration region which propagates towards the lower left corner. The first four frames of Fig. 2 show a recession of the high concentration region towards the upper right corner before the front advances towards the lower left one. Note the similarities (skew symmetry) between the first and seventh frames of Fig. 2.

Table 1

<table>
<thead>
<tr>
<th>((f, \epsilon, q))</th>
<th>((T, w, u_M, v_M))</th>
<th>((f, \epsilon, q))</th>
<th>((T, w, u_M, v_M))</th>
</tr>
</thead>
<tbody>
<tr>
<td>((1.4, 0.01, 0.002))</td>
<td>((1.61, 0.32, 0.94, 0.19))</td>
<td>((14, 0.01, 0.002))</td>
<td>((1.54, 0.64, 0.87, 0.20))</td>
</tr>
<tr>
<td>((1.4, 0.01, 0.02))</td>
<td>((1.91, 0.36, 0.81, 0.22))</td>
<td>((1.4, 0.001, 0.02))</td>
<td>(\large{\text{(A)}})</td>
</tr>
</tbody>
</table>

\(\large{\text{(A)}}\) Almost uniform concentration of \( u \). \( u(20\delta, 20\delta, t) = 2.3069 \times 10^{-3} \) for \( 90 \leq t \leq 100 \).
A detailed study of the processes observed in Fig. 2 is exhibited in Fig. 3 which indicates that the high concentration region at the upper right corner is transformed into a curved band which propagates towards the lower left corner.

For $f = 1.4$, $q = 0.02$ and $\epsilon = 0.001$, the results presented in Figs. 4 and 5 indicate the strong influence of $\epsilon$ on wave propagation in two-dimensional reactive-diffusive media. Fig. 4 shows that an almost circular front propagates from the upper right corner towards the lower left one, and that a high concentration region is observed at that corner in the eighth frame of that figure. However, a detailed study of the phenomena observed in Fig. 4 indicates that the initial almost circular front undergoes a transition to an almost planar front before reaching the diagonal that connects the upper left and lower right corners of the domain as illustrated in Fig. 5. This almost planar front changes curvature after crossing this diagonal and creates a high concentration region which moves rather quickly towards the lower left corner as illustrated in the ninth frame of Fig. 5.
Figs. 2–5 clearly show that no spiral waves are observed for $f = 1.4$ and $q = 0.02$, and $\epsilon = 0.01$, and $0.001$.

For $f = 14$, $q = 0.002$ and $\epsilon = 0.001$, it was found that $u(20\delta, 20\delta, t)$ and $u(25\delta, 20\delta, t)$ grow almost linearly with time and their values at $t = 100$ exceed $500$ and $800$, respectively, whereas $v(20\delta, 20\delta, t)$ and $v(25\delta, 20\delta, t)$ decrease almost linearly with time and their values at $t = 100$ are smaller than $-1.5 \times 10^4$ and $-4.5 \times 10^4$, respectively. For $f = 0.14$, $q = 0.002$ and $\epsilon = 0.001$, and for $f = 1.4$, $q = 0.0002$ and $\epsilon = 0.001$, it has been observed that $u(20\delta, 20\delta, t)$ and $u(25\delta, 20\delta, t)$, and $v(20\delta, 20\delta, t)$ and $v(25\delta, 20\delta, t)$ decrease almost linearly with time and their values at $t = 100$ are smaller than $-3.95 \times 10^7$ and $-1.9 \times 10^7$, respectively.

In view of the results presented in Figs. 1–5 and Table 1, it can be stated that the parameters $f$, $q$ and $\epsilon$ of the Oregonator model play a key role in determining the propagation or annihilation of spiral waves, and that these values must be restricted so as to preserve the positivity of the concentration of both the activator and the inhibitor.
The effects of the diffusion coefficients of the activator and inhibitor on spiral wave propagation in two-dimensional excitable media are summarized in Table 2. This table indicates that the separation between and the width of the pulses in $u$ and the maximum value of $u$ at $(x, y) = (20\delta, 20\delta)$ are not very sensitive to $d_v$ as this parameter is decreased from 0.6 to 0.006. However, for $d_v = 600$, a tongue-like shape which remains stationary and only occupies part of the computational domain was observed. Very large values of $d_v$, e.g., $10^5$, were found to result in unbounded negative values of $u$ and $v$. For example, the values of $u$ and $v$ at $(x, y) = (20\delta, 20\delta)$ were found to decrease almost linearly with time and were smaller than $-3.5 \times 10^8$ and $-2.45 \times 10^7$, respectively, at $t = 100$ for $(d_u, d_v) = (1, 6 \times 10^5)$. On the other hand, for small values of $d_u$, the initial profile of $u$ diffuses slowly and $u$ acquires a ring-like structure characterized by narrow stripes were the activator’s concentration is high and much wider valleys where the activator concentration is very small as shown in Fig. 6; these rings are almost concentric with the wedge type of initial conditions for the activator’s concentration (cf. Eq. (4)).
High values of $du$ result in unbounded negative values of $u$ and $v$; for example, for $(du, dv) = (10^5, 0.6)$, $u(20\delta, 20\delta, t)$ and $v(20\delta, 20\delta, t)$ decrease almost linearly with time and their values at $t = 100$ are smaller than $-3.95 \times 10^8$ and $-1.95 \times 10^8$, respectively. Moderate values of $du$, i.e., $du = 100$, result in an

Table 2
Separation ($T$) between and width ($w$) of the pulses in the activator’s concentration $u$, and maximum values of $u$ and $v$ at $(x, y) = (20\delta, 20\delta)$ as functions of $du$ and $dv$. (Unless stated otherwise $f = 1.4$, $q = 0.02$, $\epsilon = 0.001$, $L_x = L_y = 7.5$)

<table>
<thead>
<tr>
<th>$(du, dv)$</th>
<th>$(T, w, u_M, v_M)$</th>
<th>$(T, w, u_M, v_M)$</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>(1, 0.6)</td>
<td>(1, 0.006)</td>
</tr>
<tr>
<td></td>
<td>(1.60, 0.31, 0.77, 0.20)</td>
<td>(1.61, 0.29, 0.76, 0.25)</td>
</tr>
<tr>
<td>$(du, dv)$</td>
<td>(0.01, 0.6)</td>
<td>(100, 0.6)</td>
</tr>
<tr>
<td></td>
<td>(T, w, u_M, v_M)</td>
<td></td>
</tr>
<tr>
<td></td>
<td>(B)</td>
<td>(1.61, 0.37, 0.92, 0.21)</td>
</tr>
</tbody>
</table>

(A) $u(20\delta, 20\delta, t) = 2.0464 \times 10^{-3}$ for $90 \leq t \leq 100$.
(B) $u(20\delta, 20\delta, t) = 2.23 \times 10^{-3}$, $v(20\delta, 20\delta, t) = 0.118$ for $90 \leq t \leq 100$. 

Fig. 5. Concentration of the activator $u$ at (from left to right, from top to bottom) $t = 103.000$, 103.008, 103.016, 103.024, 103.032, 103.040, 103.048, 103.056 and 103.064 ($du = 1$, $dv = 0.6$, $f = 1.4$, $q = 0.02$, $\epsilon = 0.001$, $L_x = L_y = 7.5$).
almost uniform concentration of the activator throughout the whole computational domain.

It must be pointed out that shadow systems correspond to either $d_u = 1$ or $d_v = 1$ in Eq. (1) or (2), respectively, so that either the equation for $u$ or that for $v$ becomes an elliptic rather than a parabolic, partial differential equation. The results presented in Table 2 are consistent with either $d_u \to 1$ or $d_v \to 1$, for these limits correspond to large diffusion coefficients and spatially uniform concentrations of either $u$ or $v$, respectively; the limits $d_u \to 0$ or $d_v \to 0$, on the other hand, correspond to the absence of diffusion. It must be pointed out that, despite the absence of diffusion in $u$ or $v$ when $d_u = 0$ or $d_v = 0$, respectively, the values of $u$ and $v$ are nonhomogeneous because the two dependent variables are coupled in a nonlinear manner and one of them includes diffusion.

The effects of domain truncation or expansion on the propagation of spiral waves in two-dimensional reactive–diffusive media have also been investigated and a summary of the results obtained is presented in Table 3. This table shows
that the spiral wave is very robust under truncation or expansion of the computational domain as indicated by the almost constant values of the width of and the period between successive pulses of the activator’s concentration and the maximum concentrations of both the activator and the inhibitor at \((x, y) = (20\delta, 20\delta)\), and these results are in accord with the analytical ones of Sandstede [15] who proved the stability of spiral waves, the persistence of spirals and the behavior of their spectral properties under domain truncation using the spatial dynamics of elliptic (steady-state) equations.

Some sample results illustrating the effects of domain squeezing are presented in Fig. 7. This figure clearly shows the elongation of the spiral wave in

![Fig. 7. Concentration of the activator \(u\) at (from left to right, from top to bottom) \(t = 100.4, 100.6, 100.8, 101, 101.2, 101.4, 101.6, 101.8\) and 102 \((du = 1, \; d_e = 0.6, \; f = 1.4, \; q = 0.002, \; \epsilon = 0.01, \; L_x = 7.5, L_y = 5)\).]
The longest direction of the computational domain and is to be compared with that corresponding to a domain with $L_x = L_y$ [17].

The results presented in Fig. 7 do confirm the robustness of spiral waves under domain truncation or squeezing in two-dimensional reactive–diffusive media and show that the initial conditions (cf. Eqs. (4) and (5)) are forgotten and the spiral wave's tip rotates about the center of the computational domain once a periodic regime is achieved. The results presented in Fig. 7 are in marked contrast with those exhibited in Fig. 6 which show that, for small diffusion coefficients, the initial conditions play a paramount role in determining stationary patterns in two-dimensional reactive–diffusive media.

4. Conclusions

The dynamics of the two-equation Oregonator model in two-dimensional reactive–diffusive media has been studied numerically as a function of the diffusion coefficients, reaction rate parameters and dimensions of the reactive–diffusive medium, and it has been shown that spiral waves are robust under truncation or expansion of the computational domain as indicated by the almost invariance of the width and period of the activator's concentration and the maximum concentrations of both the activator and the inhibitor at two different monitoring points.

It has also been found that large diffusion coefficients for the inhibitor may result on either annihilation or unbounded growth. In the case of annihilation, it has been observed that the activator's concentration reaches very small values, whereas that of the inhibitor is of significant magnitude. Large diffusion coefficients for the activator concentration were found to result in unbounded decay of both the activator's and inhibitor's concentrations.

Small diffusion coefficients of the inhibitor resulted in stationary tongue-like shapes characterized by high concentrations of the activator, whereas small diffusion coefficients of the activator were found to result in narrow ring shapes where the activator's concentration is high.

The three parameters which govern the reaction terms in the two-equation Oregonator model have been found to play a paramount role in determining the propagation of spiral waves in two-dimensional reactive–diffusive media. A decrease in the parameter which controls the stiffness of the activator's reaction rate was found to result in unbounded growth of the concentration, whereas an increase in the parameter $f$ that couples the activator and inhibitor concentration equations was found to result in either annihilation of the spiral wave or unbounded growth of the concentrations of both the activator and the inhibitor. The third parameter was found to play an important role on the dynamics of spiral wave whenever the activator's concentration became equal to
or smaller than the value of this parameter. When this occurred, the third term in the reaction rate for the activator’s concentration changed sign and could result in unbounded growth in regions with sufficiently small activator’s concentration.

Acknowledgements

The research reported in this paper was supported by Project PB97-1086 from the D.G.E.S. and Project BFM2001-1902 de la Dirección General de Investigación of Spain and Fondos Feder.

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