Spatio-temporal patterns in excitable media with non-solenoidal flow straining

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Abstract

The propagation of spiral waves in excitable media with the Belousov–Zhabotinsky reactions in a non-solenoidal, time-independent velocity field is studied numerically as a function of the amplitude and frequency of the velocity. It is shown that the spiral wave is slightly distorted for small amplitudes and low frequencies, whereas it breaks-up into new spiral waves which merge and form periodic, cusped fronts at moderate amplitudes and small frequencies. For larger amplitudes but still small frequencies, the spiral wave undergoes a second transition to thick fronts characterized by small curvature, and the radius of curvature increases as the amplitude of the velocity field is increased. It is also shown that an increase in the frequency of the velocity field results in front distortion and corrugations which are due to the increase in the number of stagnation points as the frequency is increased, straining of the front at stagnation points and the non-solenoidal velocity field employed in the paper. An explanation of these corrugations in terms of the straining, gradient of the transverse velocity along the normal to the front and compressibility is provided. © 2001 IMACS. Published by Elsevier Science B.V. All rights reserved.

Keywords: Spatio-temporal patterns; Belousov–Zhabotinsky reactions; Ginzburg–Landau equation

1. Introduction

In a variety of spatially-extended systems, such as flames, solidification fronts, excitation waves in biological media and chemical waves, one may observe moving fronts that separate the medium in parts with different states [1–3]. The stability of such fronts is affected by both diffusive and convective transport, because transport provides the coupling between spatially separated parts of the medium. Most of the studies on the stability of fronts performed to date have been concerned with diffusive transport. However, homogeneous flows may arise naturally in systems subjected to external, e.g., electric, fields, and such fields may unequally affect the different components, e.g., ions, of the system, and, as a consequence,
the flow velocities or transport of the various components may be different. This differential flow of constituents can lead to the appearance of spatio-temporal patterns.

Excitable media may exhibit rich spatio-temporal patterns owing to their non-linearity. In this paper, we single out a peculiar feature of spiral waves, namely, their behavior under the application of a time-independent convective/advective flow field. Under these conditions, it is well-known that, in addition to its rotation, the spiral wave has a drifting motion which may be uniform in speed and direction. The drift of spiral waves has been found in heart tissue; sometimes, the drift is spontaneous due to meandering, and sometimes it is gradient-induced.

Advection may also disorganize spiral waves in Petri dishes with a surface in contact with air where convection is induced by evaporative cooling, and large convective velocities may cause sufficiently large phase gradients which may generate new spiral waves [4]. For example, for passive convection, i.e. for sufficiently important convective motions which are not very sensitive to the feedback of the chemical reactions, one can obtain a Ginzburg–Landau equation which includes advective effects, and deduce the corresponding phase dynamics equation. This equation can, in turn, be approximated as the sum of the phase in the absence of convection plus terms which account for advection. By expanding this equation in terms of the maximum speed of the convective field, i.e. by using a perturbative approach, one may obtain the horizontal phase perturbations which clearly show that the convective field disorganizes the spiral wave [5].

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 convection perturbations, and proposed a semi-empirical 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] 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. Rovinsky et al. [8] have analyzed a generalized Kuramoto–Sivashinsky equation describing the dynamics of perturbations of a planar front in systems with differential flows, i.e. the flow velocities of various components may be different, and showed that a periodic pattern of modulation may appear on the front. Kærn and Menzinger [9] considered a one-dimensional reaction–diffusion equation and a plug flow velocity, and predicted the existence of stationary waves quite different from those associated with the Turing mechanism which requires a fast inhibitor diffusion for the formation of spatially periodic patterns. The stationary waves obtained by Kærn and Menzinger [9] were also found to be quite different from those associated with differential flow instabilities.

More recently, Andresén et al. [10] considered the formation of stationary periodic patterns in the presence of a constant plug flow, and the Brusselator model, and showed that their one-dimensional model may exhibit such patterns even in the case of equal diffusion coefficients for certain types of boundary conditions in an open system. Biktashev et al. [11] considered an excitable medium moving with relative shear and the cubic FitzHugh–Nagumo equations with recovery which, in the absence of shear, would produce a pair of spiral waves when subjected to a localized disturbance. However, when subjected to shear, the spiral waves were distorted and then broken by the medium. Biktashev et al. [11] also showed that such breaks generate new spiral waves and lead to a complicated spatio-temporal pattern. Ševčíková and Müller [12] have shown experimentally that imposing an electric field on spatially-distributed chemical systems with catalytic reactions of the Belousov–Zhabotinsky type may lead to waves which propagate faster against a gradient of the electric potential and slower along it. They also showed that,
for sufficiently strong electric potentials, the Belousov–Zhabotinsky waves may split into new waves, reverse the direction of wave propagation, and/or result in wave annihilation and drift of the spiral cores.

In this paper, a numerical study of excitable media governed by the Belousov–Zhabotinsky equation in two-dimensional, stationary, convective/adveective, non-solenoidal flow fields is presented. The flow field is of the trigonometric type, and the propagation, annihilation and splitting of spiral waves in excitable media are analyzed as functions of the amplitude and frequency of the velocity field, both small and large velocities are considered. The velocity field is assumed to be the same for both the fast and slow variables, i.e. the same for both the activator and the inhibitor. Furthermore, differential flow effects due to the different diffusive fluxes owing to the different (constant) diffusivities of the slow and fast variables are considered, and these fluxes may induce spatio-temporal patterns. In addition, since the velocity field considered in this paper are not uniform, they introduce anisotropic effects which alter the shape and speed of propagation of the spiral wave.

2. Governing equations

The numerical study presented here is based on the Belousov–Zhabotinsky reaction which is often modeled by the Oregonator equations [1,2]

\[
\frac{\partial \mathbf{V}}{\partial t} + \mathbf{v} \cdot \nabla \mathbf{V} = \nabla \cdot (\mathbf{D} \nabla \mathbf{V}) + \mathbf{S},
\]

where \( t \) is time, \( \mathbf{v} = (v_x, v_y)^T \) the velocity vector with components \( v_x \) and \( v_y \) in the \( x \)- and \( y \)-directions, respectively, \( \mathbf{V} = (u, v)^T \), \( u \) and \( v \) denote the concentrations of the activator and the inhibitor, respectively, \( \mathbf{D} \) the (diagonal) diffusivity matrix with components \( d_{11} = 1 \) and \( d_{22} = 0.6 \), and [1,2]

\[
\mathbf{S} = \left( \frac{1}{\epsilon} \left( u - u^2 - fu \frac{u - q}{u + q} \right), u - v \right)^T,
\]

\( \epsilon = 0.01 \), \( f = 1.4 \) and \( q = 0.002 \). This equation was solved in the (square) domain \([-7.5, 7.5] \times [-7.5, 7.5] \) subject to homogeneous Neumann boundary conditions.

The velocity field considered here is

\[
v_x = A \cos \left( \frac{i \pi x}{L} \right) \cos \left( \frac{j \pi y}{L} \right), \quad v_y = A \cos \left( \frac{m \pi x}{L} \right) \cos \left( \frac{n \pi y}{L} \right),
\]

where \( A \) denotes the amplitude, \( i, j, m \) and \( n \) are odd integer numbers and \( L = 15 \) denotes the side of the domain. This velocity field satisfies the no-slip condition at boundaries of the domain, i.e. \( \mathbf{v} \cdot \mathbf{n} = \mathbf{v} \cdot \mathbf{t} = 0 \), where \( \mathbf{n} \) and \( \mathbf{t} \) are the unit vectors normal and tangent, respectively, to the boundary, it is not solenoidal, it is time-independent and it is not irrotational. For \( i = j = m = n \)

\[
\nabla \cdot \mathbf{v} = -A \frac{n \pi}{L} \sin \left( \frac{n \pi (x + y)}{L} \right),
\]

\[
\nabla \times \mathbf{v} = -A \frac{n \pi}{L} \sin \left( \frac{n \pi (x - y)}{L} \right) \mathbf{k},
\]
where \( \mathbf{k} \) is the unit vector normal to the \( xy \)-plane and the streamlines are straight lines with a slope equal to one.

Owing to the non-solenoidal flow field considered in this paper Eq. (1) can also be written as

\[
\frac{\partial \mathbf{V}}{\partial t} + \nabla \cdot \left( \mathbf{vV} - \mathbf{D} \nabla \mathbf{V} \right) = \mathbf{S} + \nabla \cdot \mathbf{v},
\]

and therefore, the transport (advective + diffusive flux) of the activator is different from that of the inhibitor because of the different diffusion coefficients. Moreover, this conservation equation indicates that the compressibility of the flow field modifies the (effective) reaction terms of the (original) Belousov–Zhabotinsky kinetics.

Eq. (1) was solved by means of a time-linearized, second-order accurate in both space and time method [13] which employs approximate factorization with meshes of at least, \( 102 \times 102 \) grid points and time steps equal to or smaller than 0.0001. The following initial conditions were employed in the calculations in order to establish the spiral wave within the domain

\[
u = 0 \quad \text{for} \quad 0 < \theta < 0.5, \quad u = q \frac{f + 1}{f - 1} \quad \text{elsewhere},
\]

\[
u = q \frac{f + 1}{f - 1} + \frac{\theta}{8\pi f},
\]

where \( \theta \) is the angle with respect to the origin of coordinates measured counterclockwise from the positive \( x \)-axis.

With these initial conditions and \( \nu = 0 \), calculations were performed until \( t = 20 \) in order to obtain a periodic spiral wave propagation. At \( t = 20^+ \), the velocity field was activated and the calculations were performed until \( t = 100 \).

3. Presentation and discussion of results

For the sake of conciseness, in this section we present some results corresponding to \( i = j = m = n \), i.e. \( v_x = v_y \), for different amplitudes and frequencies, i.e. different \( A \) and \( n \), of the velocity field. For \( A = 0.1 \) and \( n = 1 \), a spiral wave similar to the one observed in the absence of velocity field was observed; however, whereas the tip of the spiral wave in the absence of advection was anchored to \( x = y = 0 \), the tip of the spiral wave in the presence of the velocity field describes a closed path around the origin of coordinates as illustrated in Fig. 1. This figure clearly indicates that the spiral wave drifts in the presence of small flow velocities.

For \( A = 1 \) and \( n = 1 \), it was found that the convective field breaks the spiral into two new spiral waves which rotate in opposite directions. These waves in turn merge, create a cusped front and a finite front whose ends rotate in opposite directions and merge in a periodic manner as indicated in Fig. 2. This figure shows the periodicity of the creation of the cusped front and the merging of counter-rotating spiral waves.

For \( A = 3 \) and \( n = 1 \), very complex, time-dependent, spatio-temporal patterns were found. For \( t \leq 20 \), i.e. prior to the application of the velocity field, the spiral wave reached its characteristic rotating shape.
Fig. 1. Concentration of the activator \( u \) at (from left to right, from top to bottom) \( t = 50.4, 50.6, 50.8, 51, 51.2, 51.4, 51.6, 51.8 \) and 52 for \( A = 1 \) and \( n = 1 \).

For \( 25 \leq t \leq 44 \), the spiral wave seemed to acquire a periodic pattern characterized by a temporal period of about 1.76.

The concentrations of both the activator and the inhibitor were monitored off the origin of coordinates as functions of time, and exhibited a periodic pattern characterized by pulses of \( u \) whose amplitude and duration were about 0.886 and 0.41, respectively, and the time between two successive pulses was about 1.76. Moreover, for \( 25 \leq t \leq 44 \) similar spiral merging, reconnection, and formation of cusped fronts to those shown in Fig. 2 were observed, the cusps were sharper for \( A = 3 \) than for \( A = 1 \). At about \( t = 44 \) the periodic pattern just described underwent a transition to yet another periodic pattern characterized by pulses of the activator’s concentration whose amplitude and duration were about 0.929 and 0.460, respectively, and the separation between the pulses was about 4.35. Therefore, this transition is characterized by a higher concentration of the activator and wider and more distant pulses than the periodic pattern observed for \( 25 \leq t \leq 44 \). Moreover, the concentration of the inhibitor at the monitoring point was found to first increase sharply and then decrease slowly to a value equal to about 0.007. This periodic pattern was observed until \( t = 100 \).
The discovery of the transition of a periodic pattern to another one prompted us to perform the same calculation in a 1002 × 1002 point grid, and the results of such a calculation confirmed that such a transition was not a numerical artifact. These results are shown in Figs. 3 and 4. Fig. 3 clearly shows the spiral wave prior to the application of the velocity field (top), the wave break-up, the creation of new spiral waves and their reconnection, and the formation of a rather sharp cusped front (middle) and the annihilation of the spiral wave (bottom), whereas Fig. 4 indicates that a thick front travels from the upper left corner to the lower right corner of the domain, and the thickness of this front is comparable to the size of the domain, thus indicating that the spiral wave has undergone a transition to an almost flat and thick front. The phenomena illustrated in Fig. 4 is periodic (cf. Tables 1 and 2).

Thick almost planar fronts similar to those illustrated in Fig. 4 were also observed for \((A, n) = (5, 1)\) and \((7, 1)\), except that the second transition occurred much earlier.

For \(A = 5\) and \(n = 1\), and \(A = 7\) and \(n = 1\), thick and long fronts similar to the one shown in Fig. 4 were observed for \(t > 40\), and similar spiral break-up and reconnection to those exhibited in Fig. 3 were
obtained. However, the length and width of the fronts were larger than those of Fig. 3. The results of these calculations and others not shown here indicate that, for $A > 1$ and $n = 1$, spiral waves first break-up into new spirals which merge and form cusped fronts, and then evolve into periodic spatio-temporal patterns characterized by thick fronts of very small curvature; both the radius of curvature, and the thickness of these fronts increase as the amplitude of the velocity field increases for $n = 1$.

The effects of $n$ on spatio-temporal patterns have also been studied, and some sample results are shown in Fig. 5 which corresponds to $A = 1$ and $n = 3$; therefore, a comparison between Figs. 2 and 5 indicates the effects of the frequency of the velocity field on spiral wave propagation in excitable media. Fig. 5 indicates that the spiral wave is distorted by the velocity field, its front and back show corrugations, and its tip is not anchored at the origin of coordinates as it occurs in the absence of advection and external fields. The spiral tip describes a closed path in a periodic manner around the origin of coordinates, i.e. there is drift of the spiral wave, and this spatio-temporal pattern is periodic in both space and time.

A comparison between Fig. 1, Fig. 3 (top) and Fig. 5 indicates that the spiral wave’s length increases as $n$ increases and is less compact for $n = 3$ than for $n = 1$. Similar corrugated and meandering spiral waves...
Fig. 4. Concentration of the activator $u$ at (from left to right, from top to bottom) $t = 60, 65, 70, 75, 80, 85, 90, 95$ and $100$ for $A = 3$ and $n = 1$.

Table 1
Amplitude and duration of and separation between the pulses in the activator’s concentration, $u$, as functions of $A$ and $n$

<table>
<thead>
<tr>
<th>$A, n$</th>
<th>Amplitude</th>
<th>Duration</th>
<th>Separation</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.1, 1</td>
<td>0.777</td>
<td>0.353</td>
<td>1.647</td>
</tr>
<tr>
<td>1, 1</td>
<td>0.777</td>
<td>0.353</td>
<td>1.647</td>
</tr>
<tr>
<td>1, 3</td>
<td>0.731</td>
<td>0.460</td>
<td>1.609</td>
</tr>
<tr>
<td>1, 5</td>
<td>0.810</td>
<td>0.345</td>
<td>1.724</td>
</tr>
<tr>
<td>1, 7</td>
<td>0.789</td>
<td>0.402</td>
<td>1.609</td>
</tr>
<tr>
<td>1, 9</td>
<td>0.789</td>
<td>0.402</td>
<td>1.609</td>
</tr>
</tbody>
</table>
Table 2
Amplitude and duration of and separation between the pulses in the activator’s concentration $u$, as functions of $A$ and $n$

<table>
<thead>
<tr>
<th>$A, n$</th>
<th>Amplitude</th>
<th>Duration</th>
<th>Separation</th>
</tr>
</thead>
<tbody>
<tr>
<td>3, 1</td>
<td>0.929</td>
<td>0.743</td>
<td>4.253</td>
</tr>
<tr>
<td>3, 3</td>
<td>0.777</td>
<td>0.460</td>
<td>1.609</td>
</tr>
<tr>
<td>3, 5</td>
<td>0.823</td>
<td>0.402</td>
<td>2.011</td>
</tr>
<tr>
<td>3, 7</td>
<td>0.797</td>
<td>0.460</td>
<td>1.724</td>
</tr>
<tr>
<td>3, 9</td>
<td>0.789</td>
<td>0.460</td>
<td>1.609</td>
</tr>
<tr>
<td>5, 1</td>
<td>0.929</td>
<td>0.460</td>
<td>4.253</td>
</tr>
<tr>
<td>5, 3</td>
<td>0.760</td>
<td>0.517</td>
<td>1.724</td>
</tr>
<tr>
<td>5, 5</td>
<td>0.823</td>
<td>0.402</td>
<td>1.954</td>
</tr>
<tr>
<td>5, 7</td>
<td>0.804</td>
<td>0.402</td>
<td>1.724</td>
</tr>
<tr>
<td>5, 9</td>
<td>0.707</td>
<td>0.517</td>
<td>1.609</td>
</tr>
<tr>
<td>7, 1</td>
<td>0.929</td>
<td>0.460</td>
<td>4.253</td>
</tr>
<tr>
<td>7, 3</td>
<td>0.914</td>
<td>0.460</td>
<td>4.253</td>
</tr>
<tr>
<td>7, 5</td>
<td>0.804</td>
<td>0.345</td>
<td>1.954</td>
</tr>
<tr>
<td>7, 7</td>
<td>0.791</td>
<td>0.402</td>
<td>1.724</td>
</tr>
<tr>
<td>7, 9</td>
<td>0.707</td>
<td>0.517</td>
<td>1.609</td>
</tr>
</tbody>
</table>

to those shown in Fig. 5 have also been observed for $A = 1$, and $n = 5$, 7 and 9, except that the length of these spirals is smaller than that for $n = 3$. Moreover, the spiral wave for $n = 9$, has a similar length to that of Figs. 1 and 3 (top), thus indicating that the frequency of the velocity field plays a paramount role in determining the length and distortion of the spiral wave, i.e. the larger the frequency, the more compact the spiral wave front.

The magnitude of the distortion or spatial corrugations of the spiral wave increases as $A$ is increased as indicated in Fig. 5, and Figs. 6 and 7 which correspond to $A = 3$ and $n = 3$, and $A = 3$ and $n = 9$, respectively. The increase in the number of corrugations on the spiral wave front as $n$ increases is a consequence of the increase in the number of stagnation points, i.e. points where $v = 0$, as $n$ increases. Since, for $i = j = m = n$, the locations where $v_x = 0$ coincide with those where $v_y = 0$, and the streamlines are straight, it may be stated that the velocity gradient is largest along the streamlines at the stagnation points where convection is nil; therefore, the spiral wave is subjected to very large straining along the streamlines at the stagnation points. Straining effects can cause extinction phenomena analogous to those observed in flame propagation [14]; in excitable media, straining may cause front annihilation.

The motion in the vicinity of a point on the wave front can be resolved into a uniform translation and a rigid body rotation with angular velocity equal to $(1/2)\nabla \times v$ and a pure straining motion. The first two do not have any effect on the internal structure of a locally planar wave front, whereas the third one is described by the symmetric rate of the strain rate tensor $\varepsilon = (1/2)[(\nabla v) + (\nabla v)^T]$. For locally planar wave fronts, the most important decomposition of $\varepsilon$ at stagnation points is associated with $b = n \cdot e \cdot n$ where $n$ is the unit vector normal to the front. In a two-dimensional solenoidal stagnation point flow, the rate of change of the transverse component of velocity with transverse distance is $t \cdot e \cdot t$ where $t$ is the unit vector tangent to the front and this is equal to $-b$. This means that a decrease in the normal mass flux with distance through the front, i.e. $b < 0$, is reflected in a net transverse outflow, i.e. $t \cdot e \cdot t > 0$. In combustion theory, this outflow is referred to flame stretch [14], and the stretching can be written as
Fig. 5. Concentration of the activator \( u \) at (from left to right, from top to bottom) \( t = 50.4, 50.6, 50.8, 51, 51.2, 51.4, 51.6, 51.8 \) and 52 for \( A = 1 \) and \( n = 3 \).

\[-\mathbf{n} \cdot \nabla \times (\mathbf{v} \times \mathbf{n}) = -(\mathbf{n} \cdot \nabla)(\mathbf{v} \cdot \mathbf{n}) + \nabla \cdot \mathbf{v}.\] For the non-solenoidal velocity field employed in this paper, the last term of this expression is not nil, and, therefore, the compressibility of the velocity field contributes to the stretching of the spiral wave front.

As shown in Eq. (9), the non-solenoidal velocity field employed in this paper is equivalent to a conventional strong-conservation law equation where the original Belousov–Zhabotinsky reaction terms are modified by compressibility effects associated with the second term in the right-hand-side of Eq. (6). On the other hand, these compressibility effects also induce an outflow at the wave front which is to be added to the transverse gradient of the transverse velocity at the wave front, and causes straining. These two effects which are associated with volumetric expansion may dominate over the different diffusive transport of the activator and the inhibitor.

For \( A = 5 \) and \( n = 3 \) the spiral wave was severely distorted by the velocity field which caused large straining and local break-up of the spiral wave front followed by the formation of two counter-rotating waves very close to each other that merged and formed a cusped front which, in turn, broke up and formed new spiral waves. This process was repeated in a periodic manner. For \( A = 5 \) and \( n = 5, 7 \) and 9, the
spiral wave preserved its shape and integrity, i.e. it did not break-up into new spiral waves, but its length was shorter than for \( A = 1 \) and \( n = 5, 7 \) and 9, respectively, and the depth of the corrugations increased slightly as \( n \) was increased. Similar results were also found for \( A = 7 \) and \( n = 5, 7 \) and 9; however, for \( A = 7 \) and \( n = 3 \), the spiral wave was so severely strained, thickened and distorted by the velocity field that its width was comparable to the size of the domain employed in the calculations.

A brief summary of the calculations presented in this paper and others not shown here is presented in Tables 1 and 2 which exhibit the amplitude and duration of and the separation between the pulses of the activator concentration \( u \) at two monitoring positions off the origin of coordinates. These tables were obtained once the solution achieved a periodic pattern, and indicate that the amplitude and duration of the pulses of \( u \) are not very strong functions of \( A \) and \( n \) while the separation between the pulses is large for \( n = 1 \) and \( A = 3, 5 \) and 7, and for \( A = 7 \) and \( n = 3 \) as discussed previously. The results presented in this section and others not shown here indicate that the amplitude and frequency of non-solenoidal velocity fields influence the bifurcations of spiral waves in excitable media subjected to non-solenoidal velocity fields.
4. Conclusions

A second-order accurate in both space and time, approximate factorization, finite difference technique has been used to study the propagation of spiral waves in an excitable medium with the Belosov–Zhabotinsky reactions in a non-solenoidal, time-independent velocity field as a function of the amplitude and frequency of the velocity. The study considered the formation of a spiral wave in a (square) domain subjected to homogeneous Neumann boundary conditions, and its spatio-temporal evolution when a velocity field was applied.

The results of the study indicate that, depending on the amplitude and frequency of the velocity field, several spatio-temporal patterns ranging from spiral waves with small drift to wave break-up and reconnection, and formation of thick, almost planar fronts are possible. For small amplitudes and low frequencies, it was found that the spiral wave was slightly distorted by the velocity field, whereas it broke up into new spiral waves which merged and formed periodic, cusped shapes at moderate amplitudes and small frequencies. For larger amplitudes but still small frequencies, the spiral wave underwent a second
transition to a thick front characterized by small curvature and the radius of curvature increased as the amplitude of the velocity field was increased.

It was also found that an increase in the frequency of the velocity field resulted in front distorsion and corrugations which are due to the increase of the number stagnation points as the frequency is increased, straining of the wave front at stagnation points and the non-solenoidal velocity field employed in the calculations. An explanation of these corrugations in terms of the straining, gradient of the transverse velocity along the normal to the front and compressibility has been provided.

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