Turing pattern outside of the Turing domain

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Abstract

There are two simple solutions to reaction-diffusion systems with limit-cycle reaction kinetics, producing oscillatory behaviour. The reaction parameter μ gives rise to a 'space-invariant' solution, and μ versus the ratio of the diffusion coefficients gives rise to a 'time-invariant' solution. We consider the case where both solution types may be possible. This leads to a refinement of the Turing model of pattern formation. We add convection to the system and investigate its effect. More complex solutions arise that appear to combine the two simple solutions. The convective system sheds light on the underlying behaviour of the diffusive system.

Keywords: reaction-diffusion, limit cycle, Schnakenberg, Turing pattern, convection

1 Reaction-diffusion system

Reaction-diffusion systems can readily produce periodic behaviour. We consider such a model with limit cycle reaction kinetics:

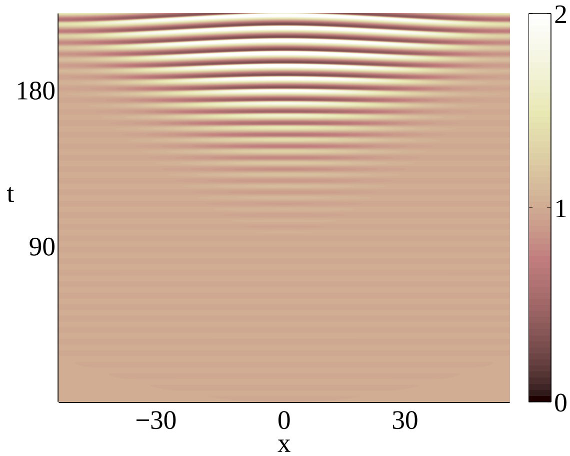
$$\begin{aligned} u_t &= \varepsilon_1 u_{xx} + f \\ v_t &= \varepsilon_2 v_{xx} + g \end{aligned} \tag{1}$$

Diffusion is an approximate model of local, uncoordinated movement (Brownian motion). We choose a particular set of reaction functions that was found by Schnakenberg [1],

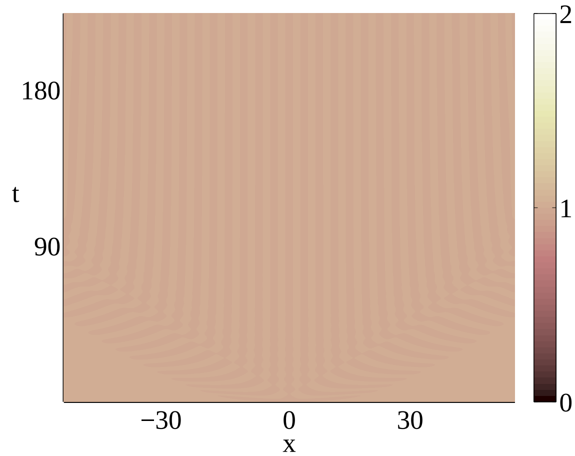
$$\begin{aligned} f &= \mu - uv^2 \\ g &= uv^2 - v \end{aligned} \tag{2}$$

Derived from a cubic-autocatalytic chemical reaction by the law of mass action, they are the algebraically simplest which can produce a limit cycle.

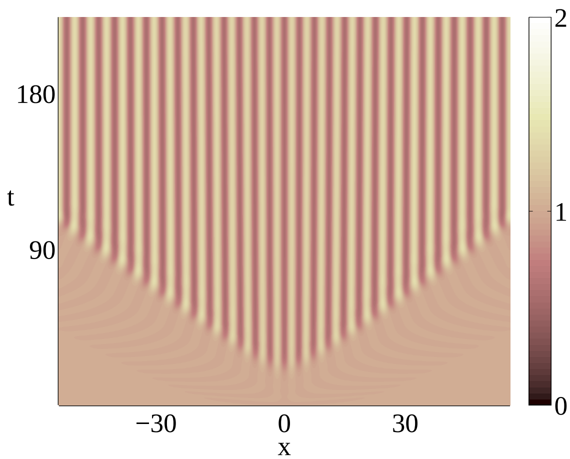
There are two distinct solutions to this problem that we can readily suggest, each one for different parameter ranges. We produce these solutions numerically, simulating an unbounded domain. A comparison of the approximate analytical solutions with their numerical counterparts is then necessary. The regions of validity are explored and tested, producing some interesting results. We discover a distinction between theory and qualitative behaviour.



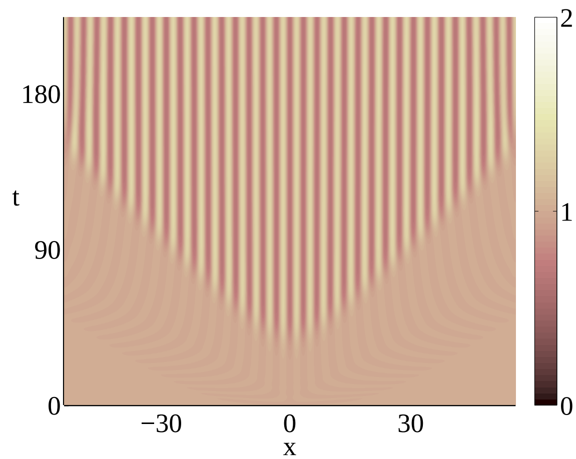
(a) ‘Space-invariant’ solution ($\mu = 0.95$, $\varepsilon_1 = \varepsilon_2 = 1.0$)



(b) Outer parameter regime ($\mu = 1.1$, $\varepsilon_1 = 1.0$, $\varepsilon_2 = 0.15$)



(c) Inner parameter regime ($\mu = 0.95$, $\varepsilon_1 = 1.0$, $\varepsilon_2 = 0.1$)



(d) Turing solution ($\mu = 1.1$, $\varepsilon_1 = 1.0$, $\varepsilon_2 = 0.1$)

Figure 1: Solutions of a diffusion model with limit cycle reaction kinetics (1). The ‘space-invariant’ ($\mu < 1$) solution (a) is close to a solution of the ODE in time, and so u_x, v_x, u_{xx} and $v_{xx} \approx 0$. It is essentially constant in space: the peaks are approximately in horizontal lines. The outer parameter regime (neither ‘space-invariant’ nor Turing) (b) shows a stable steady state, with the ghost of a Turing pattern. The Turing solution ($\left(3 - 2\sqrt{2}\right)\varepsilon_1 > \mu^2\varepsilon_2$) (d) oscillates only in space: the waves are aligned vertically. The inner parameter regime (satisfying both ‘space-invariant’ and Turing conditions) (c) shows a solution qualitatively the same as the Turing solution. The basic effect of diffusion is apparent in the outwards (both x-increasing and -decreasing) propagation of the patterns. The ‘space-invariant’ solution is slow to settle in the oscillatory mode; the Turing is less pronounced – it has a lower amplitude. The basic effect of diffusion is apparent in the outwards (both x-increasing and -decreasing) propagation of the pattern, giving the characteristic V-shape. These are numerical solutions using NAG D03PCF, plotting rescaled species $\bar{u} = \mu u$. Initially the solution is at steady state $(u, v) = (1/\mu, \mu)$, with a small disturbance at $x = 0$. At the boundary we hold the derivative at zero ($u_x = 0$, $v_x = 0$). The spatial domain is $(-56, 56)$, with a total length of 112.

1.1 'Space-invariant' solution

A simple solution is to consider a 'space-invariant' solution: $u_x \approx 0$, $v_x \approx 0$. This removes the effect of diffusion and reverts the system to the ODE, approximately:

$$\begin{aligned} u_t &\approx f \\ v_t &\approx g \end{aligned} \tag{3}$$

For μ within the parameter range for the ODE limit cycle, the PDE could then also generate a pattern, namely the ODE solution. Merkin, Needham and Scott [2] found limit cycles to exist in the ODE system for $0.90032 \approx \mu_\star < \mu < 1$. The combination of oscillations in the time-ODE, and the assumption of small variation in space ($u_x \approx 0$, $v_x \approx 0$), means that we expect oscillations to occur in time only and not in space. The pattern should look approximately like horizontal lines in a contour plot, and we find this is the case in our numerical experiment (Figure 1(a)). The effect of diffusion is apparent in the establishment of the pattern – the outwards-propagating V shape. The pattern is not entirely horizontal: there is perhaps a lag in phase outward from the centre, due to the diffusion being a secondary effect to the ODE-like behaviour. We see that this solution takes a relatively long time to settle into the oscillatory pattern.

1.2 Turing pattern

Turing found that instability can be caused by diffusion [3]. To prove this, the steady state must be stable in the absence of diffusion, and so we restrict our investigation to $\mu > 1$. To obtain this effect, we need to impose a constraint on the relative strengths of the diffusion terms. For these particular reaction functions this condition is $\left(3 - 2\sqrt{2}\right)\varepsilon_1 > \mu^2\varepsilon_2$. For example, if $\mu = 1.1$, $\varepsilon_1 = 1$ and $\varepsilon_2 = 0.1$ we can expect a Turing instability, yielding a pattern. The dramatic difference between the two diffusion rates is characteristic of this phenomenon. The strength of this constraint has raised doubts about the applicability of the model [4].

The analysis linearises the system about the steady state, then we look for a solution of the form $e^{\lambda t}\cos kx$ [5]. This form is only valid locally to the steady state, but we hope it will have some bearing on the long-term behaviour. The oscillation is in space only, not time, so the linear pattern looks like vertical lines in a contour plot. We find numerically a solution which behaves as the linear analysis suggests (Figure 1(d)). The pattern forms quickly, and apparently settles almost immediately it forms. The amplitude of this pattern is significantly less than that of the previous 'space-invariant' solution.

It is perhaps surprising that such a simple, controlled pattern occurs. The boundedness of the behaviour is a non-linear effect, related in some way to the limit cycle behaviour of the ODE. Schnakenberg chooses bounding constraints to counter global instability when selecting his functions . This is a similar concept to that employed in Poincaré-Bendixon's proof of the existence of limit cycles [6]. It seems that this bounding applies more generally in the system than the limit cycle range of the ODE. That there is a type of solution which lacks a temporal component is perhaps a fundamental property of the system.

1.3 Inner parameter regime

The Turing premise is founded on a steady state stable in the absence of diffusion. This is required principally for proof of concept – it is not utilised in the construction of the linear solution. The constraint found relating the diffusion parameters is the necessary one for instability, and hopefully pattern formation. So we choose parameters to take us inside the domain of both the 'space-invariant' and the Turing solutions. As we have seen, the general solution which is unstable in the absence of diffusion (our 'space-invariant' solution) is far removed from the Turing pattern: the two could not be confused in the numerical solution. For our inner parameters, the Turing pattern dominates to the extent of complete exclusion of the 'space-invariant' pattern (FIGURE 1(c)). This confirms that the stability requirement of Turing has no bearing on the range of the effect.

The pattern is a little stronger (the oscillations have higher amplitude) than the original Turing pattern, and the uptake is more rapid. We see too that the frequency of the waves is slightly lower. We can connect this inverse relation between amplitude and frequency if we consider that the rate of change of concentration remains within some limits.

1.4 Outer parameter regime

We consider the parameter region outside of the above solutions. There is no reason to suspect any instability, and in this respect the numerical results confirm our suspicions (FIGURE 1(b)). There is the ghost of an effect, and it looks like a Turing pattern.

2 Flow dynamics: adding convection

We now add convection to the system. If we apply convection to both species then we can use a change of coordinates to remove one of these terms. In the case of equal convection on both species, both terms are removed together and there is no perturbation to the original system: the solution is merely translated. We take the remaining convection as constant in magnitude, with strength γ. The system is now

$$\begin{aligned} u_t &= \varepsilon_1 u_{xx} + f \\ v_t &= \varepsilon_2 v_{xx} - \gamma v_x + g \end{aligned} \tag{4}$$

We investigate the effect of convection on the solutions found previously.

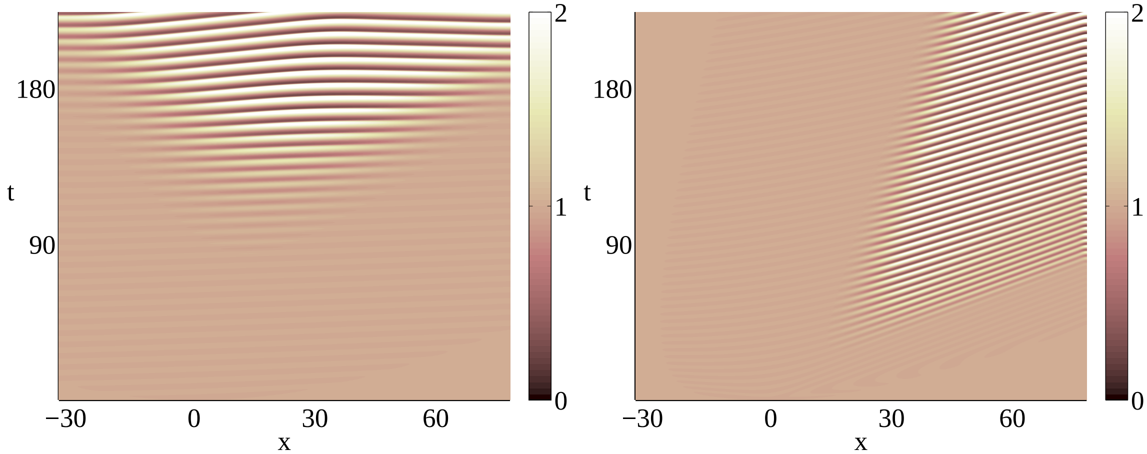
2.1 'Space-invariant' solution in the presence of convection

The 'space-invariant' solution is little affected by the addition of convection, as shown in FIGURE 2(a). The propagation is skewed by the flow, and there is some disturbance to the horizontal pattern. It seems that the uptake of the pattern is a little quicker, which gives the impression of more energy in the system.

2.2 Turing pattern, convected

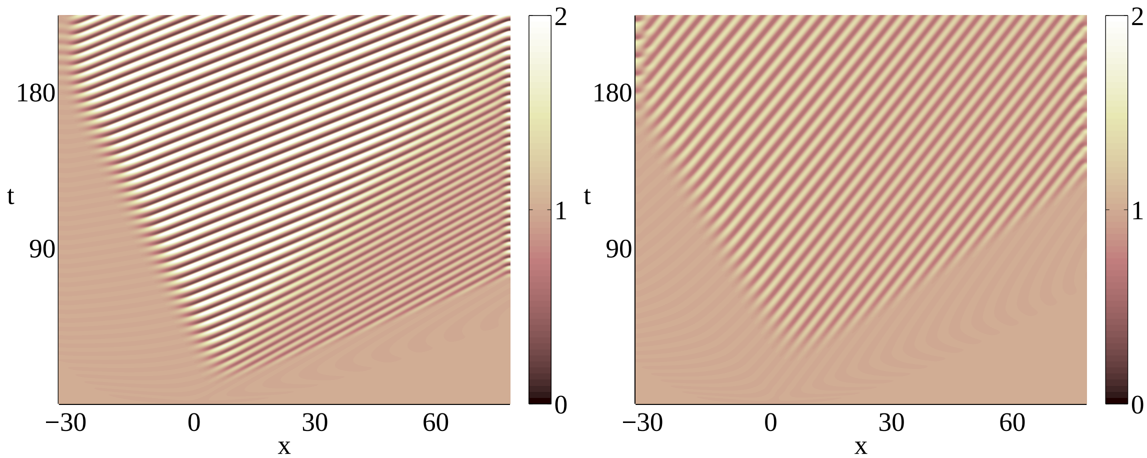
The addition of convection means that this is no longer a Turing instability; the definition does not cover the system with convection present. It is possible to generalise the concept of Turing instability to any spatial model, but the premise becomes less useful. The analysis is more complex and the demarcation of the effect more difficult to establish.

The Turing solution is substantially affected by the addition of convection (FIGURE 2(d)). The lines of constant value are no longer vertical but instead align almost exactly with the flow ($x \approx \gamma t$). The propagation is skewed more than the 'space-invariant' solution. This skewing is less dramatic than that of the alignment of the waves – perhaps at half the flow rate. Other than that, the convection has had little effect on the solution. The uptake is again rapid, and the amplitude of pattern is similar to that of the original Turing pattern.



(a) 'Space-invariance', convected ($\mu = 0.95$, $\varepsilon_1 = \varepsilon_2 = 1.0$, $\gamma = 0.3$)

(b) Outer parameter regime ($\mu = 1.1$, $\varepsilon_1 = 1.0$, $\varepsilon_2 = 0.15$, $\gamma = 1.0$)



(c) Inner parameter regime ($\mu = 0.95$, $\varepsilon_1 = 1.0$, $\varepsilon_2 = 0.1$, $\gamma = 0.7$)

(d) Turing parameters ($\mu = 1.1$, $\varepsilon_1 = 1.0$, $\varepsilon_2 = 0.1$, $\gamma = 0.3$)

Figure 2: Convective effect on pattern formation: solutions of a diffusion model with limit-cycle reaction kinetics, in the presence of convection (4). The convection has little effect on the 'space-invariant' ($\mu < 1$) solution (a). Adding convection has a dramatic effect on the Turing solution ($\left(3 - 2\sqrt{2}\right)\varepsilon_1 > \mu^2\varepsilon_2$) (d), aligning the pattern almost exactly with the flow. The inner parameter regime (satisfying both 'space-invariant' and Turing conditions) (c) shows a solution with different behaviours to left and right. The left side is similar to the 'space-invariant' solution, the right like the Turing solution. The outer parameter regime (neither 'space-invariant' nor Turing) (b) demonstrates a weaker form of the inner parameter regime. The basic effect of diffusion remains apparent in the outwards (both x-increasing and -decreasing) propagation of the pattern, with the characteristic V-shape 'pushed over' by the convection. These are numerical solutions using NAG D03PCF, plotting rescaled species $\bar{u} = \mu u$. Initially the solution is at steady state $(u, v) = (1/\mu, \mu)$, with a small disturbance at $x = 0$. At the boundary we hold the derivative at zero ($u_x = 0$, $v_x = 0$). The spatial domain is $(-33.6, 78.4)$, with a total length of 112, as before.

2.3 Inner parameter regime

In this situation we can be confident of interesting behaviour. We have the conjunction of the two types of instability with the potentially destabilising effect of convection. The numerical results satisfy our expectations (FIGURE 2(c)). There is a strong, clear pattern formed, with a distinctly new conformation. The pattern has two distinct sides to it, with a clear demarcation between them. The right side is reminiscent of the convected Turing pattern, and the left more like the 'space-invariant' convected pattern.

2.4 Outer parameter regime with convection

With a little convection ($\gamma = 0.3$), there is no noticeable creation of pattern. This seems reasonable since, without convection, we are in a stable parameter regime. When we add a more substantial amount of convection ($\gamma = 1.0$) we see a pattern emerge (FIGURE 2(b)). This type of numerical solution was first discovered by Satnoianu, Merkin and Scott [7].

The pattern is similar to the convected solution inside both parameter ranges. It again has aspects of the convected form of both the 'space-invariant' and Turing solutions. The pattern aligns strongly with the convection, similar to the convected Turing pattern. The uptake of the pattern is rapid, again like the Turing pattern. There are two areas of the pattern, the right and left, with the left much more extensive. The left is strong like the 'space-invariant' solution, the right weaker like the Turing pattern. The existence of different behaviour to right and left was found previously in the convected 'space-invariant' solution. The types of behaviour to the right and the left also coincide with the convected inner parameter regime.

3 Conclusion

We have made the distinction between the Turing proposal and the Turing effect: the effect has a broader existence than the consideration of the theory. We have shown that the general convective effect is a combination of the two simpler solutions ('space-invariant' and Turing pattern, both convected). Alternatively, the more complex convective pattern is a general solution, with the 'space-invariant' and Turing patterns demonstrating extremal behaviour of this solution. Further, we have demonstrated qualitatively a principle of addition of instabilities resulting in increase in pattern. We see that introducing convection has illuminated our understanding of the standard system.

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