Pattern Formation in Active Fluids: Turing and Beyond

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A dissertation submitted for the partial fulfillment of
BS-MS dual degree in Science

Indian Institute of Science Education and Research Mohali
April 2018

Certificate of Examination

This is to certify that the dissertation titled **Pattern Formation In Active Fluids: Turing and Beyond** submitted by **Ms. Madhuvanthi G Athani (Reg. No. MS13113)** for the partial fulfillment of BS-MS dual degree programme of the Institute, has been examined by the thesis committee duly appointed by the Institute. The committee finds the work done by the candidate satisfactory and recommends that the report be accepted.

Prof. Sudeshna Sinha	Dr. Satyajit Jena	Dr. Abhishek Chaudhuri (Supervisor)

Dated: April 20, 2018

Declaration

The work presented in this dissertation has been carried out by me with Dr. Abhishek Chaudhuri at the Indian Institute of Science Education and Research Mohali. This work has not been submitted in part or in full for a degree, a diploma, or a fellowship to any other university or institute. Whenever contributions of others are involved, every effort is made to indicate this clearly, with due acknowledgement of collaborative research and discussions. This thesis is a bonafide record of original work done by me and all sources listed within have been detailed in the bibliography.

Madhuvanthi G Athani
(Candidate)

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In my capacity as the supervisor of the candidate's project work, I certify that the above statements by the candidate are true to the best of my knowledge.

Dr. Abhishek Chaudhuri
(Supervisor)

Acknowledgements

I would like to thank my thesis supervisor Dr. Abhishek Chaudhuri for giving me the opportunity to learn and work under his guidance, for always encouraging me, making me smile, and being a constant support throughout the duration of my project.

I would also like to thank my thesis committee members, Prof. Sudeshna Sinha and Dr. Satyajit Jena for giving their valuable suggestions to the work. I would like to thank Dr. Rajeev Kapri for the constructive discussions I had with him, as I learnt news methods to approach a problem. I would like to extend my sincere gratitude to Amir from Institute of Physics Bhubaneswar, for taking the time to correct some of my mistakes and guiding me when I was stuck. I would like to thank Naveen, Mushir and Vishnu for helping me in making some plots and video clips in GNU Plot and MATLAB and my group members specially Aman for all the helpful discussions.

My time in IISER Mohali would not have been this joyful, if not for my great friends (*Othlas*, batchmates and others), who have always been there to motivate me as well as offer their criticism when needed, and so I will always be indebted to them. I would also like to thank my family for their support and the trust they have in me. Finally, I thank IISER Mohali for all the facilities and DST-INSPIRE for the financial support.

Madhuvanthi G Athani

Contents

List of Figures

Dedicated to all my friends and family

Abstract

The work at present incorporates mechano-chemical effects to extend Alan Turing's hypothesis on pattern formation. The patterns here are formed because the active stress gradients driving the hydrodynamic flows advect the stress regulator which balances out the diffusive fluxes. The first part of the work considers a mechanism where one diffusing species, in one dimension, is seen to up-regulate the active stress, which results in pattern formation. In the second part of the work two chemical species are considered in one dimension where the fast-diffusing species is taken as an up-regulator of the active stress and the slow-diffusing species is taken as a down-regulator of the active stress. Here, spontaneous pulsatory patterns are seen to emerge. This work can also be extended to higher dimensions. The entire work is based on two PRL papers cited in the reference.

Chapter 1

Introduction

Patterns are seen everywhere around us. In biological systems, colourful patterns can be found as stripes on tigers and zebras, and spots on leopards. One can also find interesting patterns on the bodies of various fishes. The ubiquitous nature of these pattern types, and what might be the underlying physical and mathematical basis of such patterns, caught the attention of many theorists. Alan Turing, the pioneer in this field of research, published a paper in 1952 titled 'The Chemical Basis of Morphogenesis' [1] where he tried to explain how patterns are formed during morphogenesis, which is the process of formation of various structures in an organism after an embryo gets formed.

1.1 Turing Patterns

It has been argued and agreed upon that spatial inhomogeneity is a pre-requisite for a growing embryo to take shape. So it is reasonable to assume that the biological signals that regulate such inhomogeneties, must themselves have an inhomogeneous spatial distribution. Hence, these biological signals operate in a concentration-dependent manner - Higher the concentration of a chemical species, greater the signal. These chemical species which determine the fate of growing cells in the context of morphogenesis are termed as Morphogens. The word 'patterns' in our present context refers to this spatial distribution of chemical species.

The mathematical model of a growing embryo needs the description of the 'state of a system' which is determined from the information of the state a short while before. The description of such a state according to Turing [1] consists of two parts:

- Mechanical Part: Information regarding stress, velocity, density, elasticity and so on.
- Chemical Part: Information on chemical reactions and on concentrations and diffusibilities of each substance at each point in time.

The mechanical and the chemical parts are most of the times coupled and this adds complexity to the problem. Turing investigated the system where the mechanical aspects can be ignored compared to the chemical aspects.

1.2 Reaction-Diffusion system

The plausible mechanism given by Turing are in terms of Reaction-Diffusion equations, where a minimum of two chemical species is considered and they are considered to be diffusing as well as reacting with each other [2].

Consider a Chemical species i with diffusion coefficient D_i. Let the concentration, a function of position x and time t, be $c_i(x,t)$. Then the flux of species i in the x-direction due to diffusion, j_i is given by:

$$\partial_t c_i = -\partial_x j_i \qquad\qquad j = -D_i \partial_x c_i \tag{1.1}$$

Let $r_i(c_i)$ be the rate of change of the species i by chemical reactions. Then the rate of change of concentration due to chemical reactions is given by:

$$\partial_t c_i = r_i(c_i) \tag{1.2}$$

If we also include diffusion of these chemical species, then we get the following Reaction-Diffusion master equation:

$$\frac{\partial c_i}{\partial t} = D_i \frac{\partial^2 c_i}{\partial x^2} + r_i(c_i) \tag{1.3}$$

This can also be generalized to two or three dimensions and multiple chemical species

$$\frac{\partial c_i}{\partial t} = D_i \bigtriangledown^2 c_i + r_i(c_i) \tag{1.4}$$

1.3 Turing System: Linear Stability Analysis

To see when the Turing system will produce spontaneous patterns, we need to do a linear stability analysis and get the conditions necessary for getting instabilities which generates patterns. Consider a one dimensional system with two chemical species. Let their concentrations be represented by a and s [3]:

$$\frac{\partial a}{\partial t} = D_a \frac{\partial^2 a}{\partial x^2} + r_a(a, s) \tag{1.5}$$

$$\frac{\partial s}{\partial t} = D_s \frac{\partial^2 s}{\partial x^2} + r_a(a, s) \tag{1.6}$$

The homogeneous steady state is (a_0, s_0) considering a perturbation about this steady state and expanding both the equations about this point, using Taylor series, where $r_{as} = \frac{\partial r_a}{\partial s}$ and $d = \frac{D_a}{D_s}$, we get:

$$\frac{\partial(a_0 + \delta a)}{\partial t} = \frac{d\partial^2(a_0 + \delta a)}{\partial x^2} + r_a(a_0, s_0) + r_{aa}\delta a + r_{as}\delta s \tag{1.7}$$

$$\frac{\partial(s_0 + \delta s)}{\partial t} = \frac{\partial^2(s_0 + \delta s)}{\partial x^2} + r_s(a_0, s_0) + r_{sa}\delta a + r_{ss}\delta s \tag{1.8}$$

Taking the spatial variation in the perturbation, as a Fourier series we get $\delta a_k(t)e^{ikx}$ with k being the mode. Now solving the differential equation, we get:

$$\frac{\partial(\delta a_k)}{\partial t} = -dk^2\delta a_k \ + r_{aa}\delta a_k + r_{as}\delta s_k \tag{1.9}$$

$$\frac{\partial(\delta s_k)}{\partial t} = -k^2 \delta s_k \ + r_{sa} \delta a_k + r_{ss} \delta s_k \tag{1.10}$$

Now we can write this in the matrix form as:

$$\frac{\partial}{\partial t} \begin{pmatrix} \delta a_k \\ \delta s_k \end{pmatrix} = \mathbf{A} \begin{pmatrix} \delta a_k \\ \delta s_k \end{pmatrix}, \qquad \mathbf{A} = \begin{pmatrix} -dk^2 + r_{aa} & r_{as} \\ r_{sa} & -k^2 + r_{ss} \end{pmatrix} \tag{1.11}$$

This is an eigenvalue equation and we will get two eigenvalues σ_1 and σ_2 and two linearly independent eigenvectors $\mathbf{V_1}$ and $\mathbf{V_2}$

$$\begin{pmatrix} \delta a_k \\ \delta s_k \end{pmatrix} = c_1 \mathbf{V_1} e^{\sigma_1 t} + c_2 \mathbf{V_2} e^{\sigma_2 t} \tag{1.12}$$

The system of equations is stable if and only if both the eigenvalues are negative. Otherwise the corresponding mode will grow and cause instabilities which will lead to spontaneous pattern formation. The eigenvalues are given by:

$$\sigma = \frac{1}{2}(tr\mathbf{A} \pm \sqrt{tr^2\mathbf{A} - 4det\mathbf{A}}) \tag{1.13}$$

Therefore the stability conditions are $tr\mathbf{A} < 0$ and $det\mathbf{A} > 0$

$$tr\mathbf{A} = -(1+d)k^2 + r_{aa} + rss \tag{1.14}$$

$$det\mathbf{A} = dk^4 - (r_{aa} + dr_{ss})k^2 + r_{aa}r_{ss} - r_{as}r_{sa} \tag{1.15}$$

Implications of this stability conditions are:

- If there is no diffusion, then $tr\mathbf{A} < 0$ if and only if r_{aa} and r_{ss} are negative. This means that the chemical reaction system by itself is stable. Trace is maximum for the zeroth mode, which means that if the instability has to occur in the trace, then the zeroth mode will be the fastest growing mode.
- If the determinant is positive at the onset of instability (when trace crosses zero) then the eigenvalues we get will be imaginary, which means that the zeroth mode is oscillatory and this leads to a Hopf bifurcation.

In the developmental context, we would want stable chemical reactions and patterns to emerge as the embryo grows, so a Hopf bifurcation is not desired. Which means at least one of r_{aa} or r_{ss} is negative. Now, without diffusion the chemical reaction is stable if $r_{aa}r_{ss} - r_{as}r_{sa} > 0$. To find the fastest growing mode in the instability, we take the differential of $det\mathbf{A}$ with respect to k^2 to get:

$$k_0^2 = \frac{r_{aa} + dr_{ss}}{2d} \tag{1.16}$$

Physical implications of the stability conditions (Turing's Condition for pattern formation):

1. The minimum occurs for a real k_0 only when there is a positive feedback present. This means that one of the chemical species must be auto-catalytic in nature. Making an arbitrary choice, let $r_{aa} > 0$ (activator). But both cannot be auto-catalytic, (to avoid Hopf bifurcation) and hence $r_{ss} < 0$ (inhibitor).
2. A further condition comes out that $d < 1$. Which means that the inhibitory species must be fast diffusing compared to the activator species.

Intuitively, we can see that the concentration of the activator builds up locally, and tries to spread. But the inhibitor spreads faster, which pins the peaks of the activator and does not let it spread. This also sets a wavelength for the pattern of the formed peaks.

1.4 What next?

In a developmental context, the spatial distribution of chemical species forms the famous Turing patterns following the reaction diffusion equations. Alan Turing in his paper in 1952, also predicted that the mechanical effects have a huge hand in pattern formation, but did not investigate it. After nearly 60 years, a major break-through happened in this field where these said mechanical effects were investigated. The work in this thesis largely is based on these two major PRL papers [4] and [5]. In the next few chapters, these mechanical effects will be investigated and some numerical results will also be presented to show pattern formation without invoking any chemical reactions.

First, we will investigate how these mechanical effects can be brought into the problem. Here we will use only one chemical species and solve the problem in one dimension. Stationary stable patterns will be seen to emerge in this situation. Next two chemical species will be considered, and oscillatory patterns will be seen after this, the model will be extended to two dimensions.

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Chapter 2

Active Fluid With One Chemical Species

It was possible to incorporate the mechanical aspects in pattern formation with the rise of the field of Active Matter. Typically in every cell, there is a mesh-work of filamentous protein structures called cytoskeletal filaments or actin materials (F-Actin). The actin helps certain other proteins called myosin motors to carry cargo across the cell [1]. The movement of myosin motors along the actin filaments causes mechanical stress on long length scales reaching up to cellular and tissue scales. This self propelled motion of the myosin motors is termed as active transport because it requires energy which comes from the hydrolysis of Adenosine Triphosphate (ATP) in cells. The system we consider here is hence, a non-equilibrium system as it is driven out of equilibrium because the system gets energy from ATP and so it is classified under a new class of materials called Active Matter [2] [3].

2.1 Advection-Diffusion Equation

The mathematical model that incorporates the mechano-chemical aspects into pattern formation was first given by Justin Bois, Frank Jlicher and Stephan Grill in 2011 [4]. This approach takes the help of an advection-diffusion equation to model the concentrations and the velocities are modelled using a force balance equation which contains a stress term. This stress term is composed of a viscosity-dependent passive stress and a concentration dependent active stress. This active stress is the contribution from the active (ATP consuming) acto-myosin components and this term is also seen to couple the velocity equation to the concentration equation.

Consider a thin film of constant thickness of the active fluid (Cytoskeleton).The movement is assumed to be solely along x-axis. The concentration $c(x,t)$ of the regulator is given by the continuity equation with j being the flux. This equation is essentially a statement of conservation.

$$\partial_t c = -\partial_x j, \qquad\qquad j = -D\partial_x c + vc \tag{2.1}$$

As the concentration flows with the fluid (moving with velocity v), the flux of the regulator has an advective component, in addition to a diffusive component (diffusion coefficient D). Since the fluid is considered explicitly here, we need to consider the corresponding constitutive equation which gives the stress as:

$$\sigma = \eta\partial_x v + (\zeta\Delta\mu)_0 f(c) \tag{2.2}$$

$\eta\partial_x v$: Passive viscous stress (η: viscosity)
$(\zeta\Delta\mu)_0 f(c)$: Active concentration-dependent stress

The active component of stress contains $\Delta\mu$ which is the change in chemical potential associated with the ATP hydrolysis and a constant ζ. $f(c)$ is a dimensionless function dependent on the concentration.

The Langevin equation, which is essentially a force balance equation, in the absence of any inertial forces, is given by:

$$\partial_x \sigma = \gamma v \tag{2.3}$$

with γ being the frictional coefficient representing the friction due to a movement over a cell membrane or a substrate.

The dimensionless function that is dependent on concentration is taken as $f(c) = \frac{c}{1+c}$. This particular form is considered because: For small values of c the function depends on this concentration, where as for large values, where $(c+1) \approx c$, $f(c)$ will approach one. Substituting this form for $f(c)$, into the equation (2.2) we get the stress to be dependent on the concentration as follows:

$$\sigma = \eta \partial_x v + (\zeta \Delta\mu)_0 \left(\frac{c}{1+c} \right) \tag{2.4}$$

Substituting (2.4) into the force balance equation (2.3) we see that the velocity is dependent on the concentration of the regulator.

$$\eta \frac{\partial^2 v}{\partial x^2} + (\zeta \Delta\mu)_0 \frac{\partial}{\partial x} \left(\frac{c}{1+c} \right) = \gamma v \tag{2.5}$$

Equation (2.1) when simplified leads to an advection-diffusion equation as follows:

$$\frac{\partial c}{\partial t} + \frac{\partial (vc)}{\partial x} = D \frac{\partial^2 c}{\partial x^2} \tag{2.6}$$

The two equations above (2.5) and (2.6) are the governing equations responsible for pattern formation. These equations were non-dimensionalized and numerically solved to obtain the patterns in one dimension.

2.2 Linear Stability Analysis

To understand the spontaneous emergence of patterns from a unique homogeneous steady state $[c(x) = c_0, v = 0]$ linear stability analysis is done considering the perturbations about these steady states [4]. Let the perturbations be of the form:

$$v = \delta v_0 e^{\beta t} e^{ikx} \qquad\qquad c = c_0 + \delta c_0 e^{\beta t} e^{ikx} \tag{2.7}$$

where the wave number corresponding to periodic boundary conditions is $k_n = \frac{2\pi n}{L}$ with $n \in \mathbb{N}$ [5]. Linearizing the system we get:

$$-k^2 \delta v_0 + ikf'(c_0) = \delta v_0 \tag{2.8}$$

$$\beta \delta c_0 + ik(pe)c_0 \delta c_0 = -k^2 c_0 \tag{2.9}$$

From the equation (2.8), solving for δv_0

$$\delta v_0 = \frac{ikf'(c_0)\delta c_0}{1+k^2} \tag{2.10}$$

Substituting (2.10) and $f'(c_0) = \frac{1}{(1+c_0)^2}$ in (2.9) and solving for β we get:

$$\beta = -k^2 \left[1 - pe \frac{c_0}{(1+k^2)(1+c_0)^2} \right] \tag{2.11}$$

where β is the growth rate of the perturbation with wave number k. Patterns spontaneously form when the uniform steady state becomes unstable, which is when the growth rate β becomes positive for some k. So the condition for pattern-forming instability on a periodic domain with $k = \frac{2\pi}{L}$ (L being the domain length) and c_0 being the uniform steady state concentration is as follows:

$$pe > \left(1 + \frac{4\pi^2}{L^2}\right) \frac{(1+c_0)^2}{c_0} \tag{2.12}$$

If the limit of a large domain size, which is when the domain size is much larger than the size of the characteristic wavelength of the instability, the condition necessary then becomes:

$$pe > \frac{(1+c_0)^2}{c_0} \tag{2.13}$$

The above is the condition for the peclet number, so that spontaneous patterns emerge. It is also important to note that the total amount of regulator is conserved, which means when there is an accumulation of concentration at a particular place, there has to be a depletion of concentration at another place.

2.3 Numerical Solution and Analysis

Let us consider that $x \in [0, L]$. After making the main equations (2.5) and (2.6) dimensionless we get:

$$\frac{\partial c}{\partial T} + pe\frac{\partial (Vc)}{\partial X} = \frac{\partial^2 c}{\partial X^2} \tag{2.14}$$

$$\frac{\partial^2 V}{\partial X^2} + \frac{\partial}{\partial X}\left(\frac{c}{1+c}\right) = V \tag{2.15}$$

where $T = \frac{t}{\tau}$ with $\tau = \frac{l^2}{D}$, $X = \frac{x}{l}$ and $V = \frac{v}{U}$. Peclet number $pe = \frac{Ul}{D}$ is the ratio of the diffusive to advective time scales. $U = \frac{(\zeta\Delta\mu)_0}{\sqrt{\eta\gamma}}$ denotes the characteristic velocity, as evident from the main equations.

Numerically solving the above equations (2.14) and (2.15) in MATLAB by following the discretization as shown in Appendix-A, the following plots were generated when periodic boundary conditions were imposed.

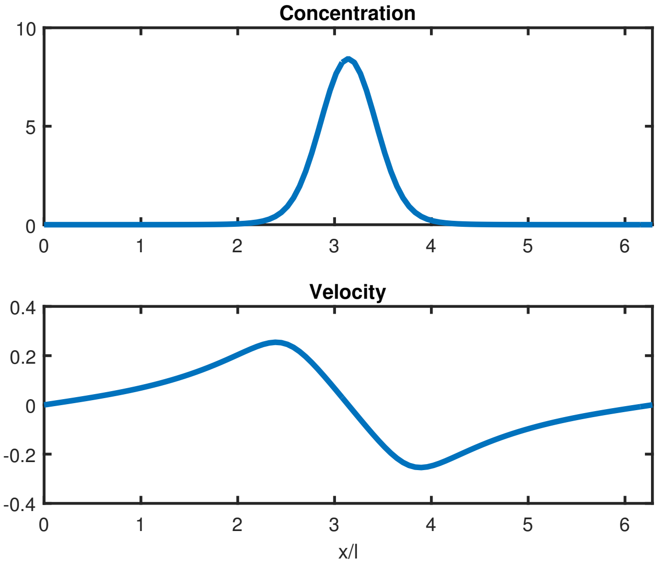

FIGURE 2.1: Concentration and Velocity (v/U) plots for $x/l = 2\pi$.

Figure 2.1 shows the non-homogeneous steady states with peclet number $pe = 25$. It can be seen that the velocity profile crosses zero, at the peak of the concentration profile. This means that the material is flowing towards the peaks and away from the valleys. Hence, the pattern is maintained by a balance of the advective flux which brings things into the peaks and the diffusive flux which take things out of them, thereby creating a concentration pattern with a steady state flow profile.

The velocity profile can be seen to cross zero at the extrema of the concentration profile such that material flows into the peaks and out of valleys. The pattern is maintained by a balance of advective flux into the peaks and diffusive flux out of them,

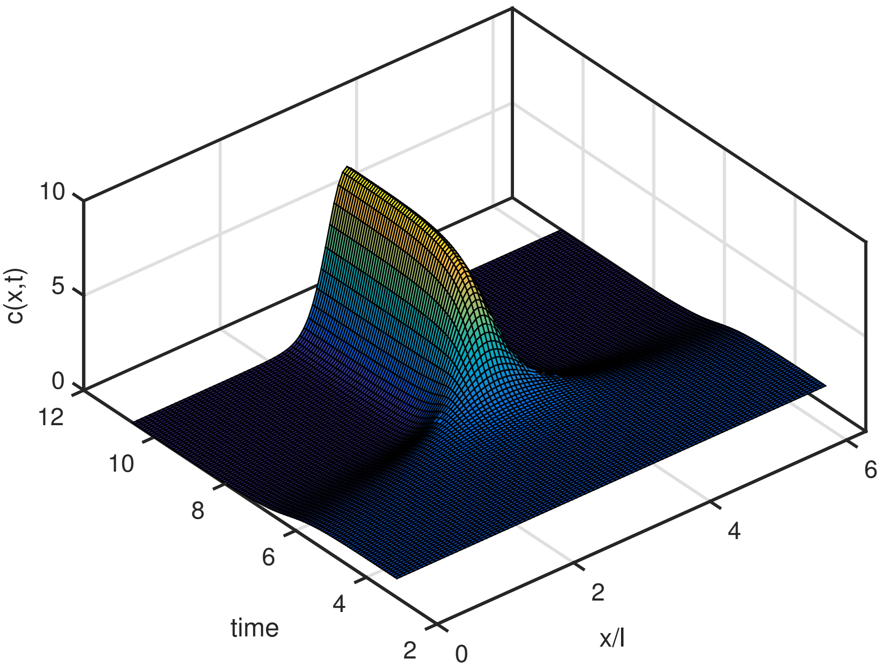

FIGURE 2.2: Spontaneous emergence of a concentration peak.

Figure 2.2 shows a spontaneous emergence of a concentration peak (pattern). Time here refers to the non-dimensionalized $T = \frac{t}{\tau}$

In the figure 2.3 an intermediate multi-peaked state can be seen. This after further evolution of time merges into a single peak which is the steady state solution. This merging can be seen clearly in the figure 2.4.

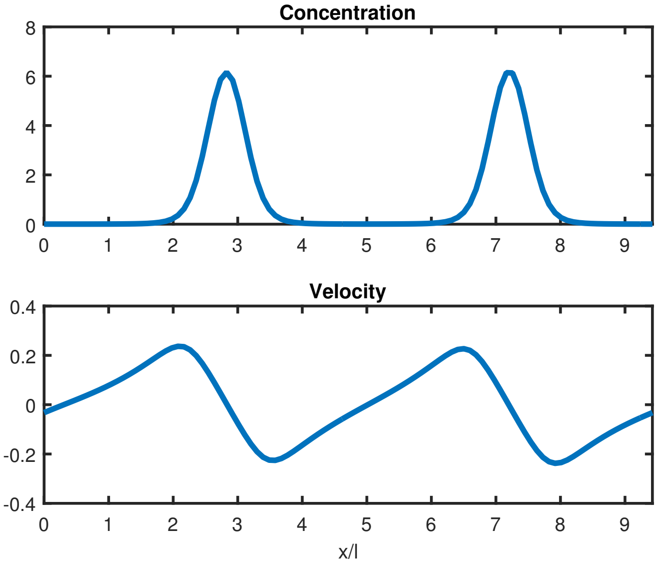

FIGURE 2.3: Intermediate multi-peaked state. Here $x/l = 3\pi$

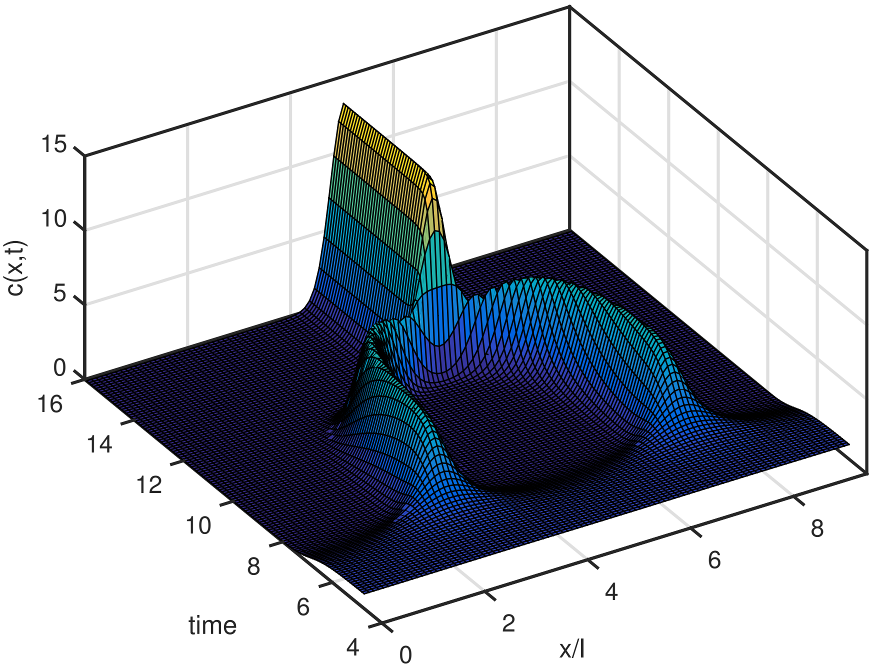

FIGURE 2.4: Merging of two intermediate peaks to form a single stable peak.

2.4 Conclusions

It was seen through linear stability analysis that the system of advection-diffusion equations considered here, should give rise to an instability and hence spontaneous patterns must emerge. This was confirmed by solving the set of these equations numerically. Hence it was shown that, even in the absence of any chemical reactions, spontaneous patterns can emerge in a system with only one diffusing chemical species (Turing system needs a minimum of two chemical species). The next question of interest would be whether such similar patterns would emerge, when multiple chemical species are involved, and if that result can also be obtained without invoking any chemical reactions.

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Chapter 3

Active Fluid With Two Chemical Species

In the presence of multiple chemical species, classical Turing instabilities could give rise to spatially periodic oscillatory patterns. Here, we ask if in an active fluid with two diffusing chemical species, the same phenomenon is observed without invoking the chemical reactions [1].

3.1 Advection-Diffusion Equation

Consider two chemical species of concentration $A(x, t)$ and $I(x, t)$ at position x and at time t, moving in a fluid of finite size L. The movement is considered to be only along the $x-$axis. The continuity equation, which considers diffusion, with diffusion coefficient D and bulk velocity v is given below:

$$\frac{\partial A}{\partial t} + \frac{\partial (vA)}{\partial x} = D\frac{\partial^2 A}{\partial x^2} \tag{3.1}$$

$$\frac{\partial I}{\partial t} + \frac{\partial (vI)}{\partial x} = \alpha D\frac{\partial^2 I}{\partial x^2} \tag{3.2}$$

Both the chemical species are diffusing with different rates of diffusion. Here $\alpha > 0$ is the ratio of the coefficients of diffusion of species I to species A. The stress has a passive term and an active term as it did in the case of a single diffusing species. This active term has contributions from both the chemical species and is given as follows:

$$\sigma = \eta\partial_x v + (\zeta\Delta\mu)_0 f(c) \tag{3.3}$$

$\eta\partial_x v$: Passive viscous stress [2] (η: viscosity)

$(\zeta\Delta\mu)_0 f(c)$: Active concentration-dependent stress

where both the chemical species A and I regulate $f(c)$

$$f(c) = (1+\beta)\frac{A}{1+A} + (1-\beta)\frac{I}{1+I} \tag{3.4}$$

Considering the equation for force balance (2.3) as in the previous case we get:

$$\eta\frac{\partial^2 v}{\partial x^2} + (\zeta\Delta\mu)_0\frac{\partial}{\partial x}\left((1+\beta)\frac{A}{1+A} + (1-\beta)\frac{I}{1+I}\right) = \gamma v \tag{3.5}$$

Equations (3.1), (3.2) and (3.5) are the main governing equations for this particular system. Note that the concentrations of both these two chemical species A and I will be conserved.

3.2 Linear Stability Analysis

To understand the dynamics of the system better, a small perturbation $\delta c = c - c_0 = e^{ikx}$ is taken about the homogeneous state $c_0 = (A_0, I_0)$, $v = 0$. Taking equation (3.5) into Fourier space, we get:

$$v_k = \frac{1}{\gamma}(\eta(ik)^2 v_k) + \frac{(\zeta\Delta\mu)_0}{\gamma}F[\partial_x f(c)] \tag{3.6}$$

where $F[\partial_x f(c)] = ik(A_k\partial_A f + I_k\partial_I f)$. Therefore v_k is given by:

$$v_k = \frac{ik(\zeta\Delta\mu)_0(A_k\partial_A f + I_k\partial_I f)}{\gamma(1 + l^2K^2)} \tag{3.7}$$

where $l^2 = \frac{\eta}{\gamma}$. Writing the equations (3.1) and (3.2) also in the Fourier space, we get:

$$\partial_t A_k = -ikv_k A_0 - Dk^2 A_k \tag{3.8}$$

$$\partial_t I_k = -ikv_k I_0 - \alpha Dk^2 I_k \tag{3.9}$$

Substituting for v_k from (3.7) into equations (3.8) and (3.9), and writing it in matrix form where **L** is the linear stability matrix we get the eigen value equation:

$$\frac{\partial}{\partial t}\begin{pmatrix} A_k \\ I_k \end{pmatrix} = \mathbf{L}\begin{pmatrix} A_k \\ I_k \end{pmatrix} \tag{3.10}$$

Let $pe = \frac{(\zeta\Delta\mu)_0}{\gamma D}$ be the peclet number, $\tau = \frac{l^2}{D}$ be the diffusive time scale, $f_A \equiv \partial_A f(c_0)$ and $f_I \equiv \partial_I f(c_0)$. The linear stability matrix (**L**) is given by:

$$\tau\mathbf{L} = -k^2l^2\begin{pmatrix} 1 & 0 \\ 0 & \alpha \end{pmatrix} + \frac{(Pe)k^2l^2}{1+k^2l^2}\begin{pmatrix} A_0 f_A & A_0 f_I \\ I_0 f_A & I_0 f_I \end{pmatrix} \tag{3.11}$$

The homogeneous state (c_0)is unstable if the leading eigen value ($\lambda_+(k)$) for the wave number k of the linear stability matrix **L** is positive. The eigen values are given by:

$$\lambda(k) = \frac{1}{2}\left[tr(\mathbf{L}) \pm \sqrt{(tr\mathbf{L})^2 - 4det(\mathbf{L})}\right] \tag{3.12}$$

where the trace is $tr\mathbf{L}$ and $\Delta\mathbf{L} = [(tr\mathbf{L})^2 - 4det(\mathbf{L})]$ is the discriminant, with $det(\mathbf{L})$ being the determinant.

$$tr\mathbf{L} = -Dk^2\left[(1+\alpha) - \frac{pe(A_0 f_A + I_0 f_I)}{1+k^2l^2}\right] \tag{3.13}$$

$$\Delta\mathbf{L} = D^2k^4\left[(1+\alpha)^2 + \frac{(pe)^2}{(1+k^2l^2)^2}(A_0 f_A + I_0 f_I)^2 - \frac{2(pe)(1-\alpha)}{1+k^2l^2}(A_0 f_A - I_0 f_I)\right] \tag{3.14}$$

For a system of size L the wave number for the periodic boundary condition is given by $k_n = \frac{2n\pi}{L}$ where $n \in \mathbb{Z}$. The mode k_1 becomes unstable when the peclet number is increased beyond the critical peclet number (pe_c). It was seen that the instabilities can be of two types - Oscillatory and Stationary. On increasing the peclet number, the homogeneous state (A_0, I_0) will undergo an oscillatory instability when $tr\mathbf{L} > 0$ and $\Delta\mathbf{L} < 0$ and this happens when $pe > pe_c$

- if $f_A > 0$ and $f_I < 0$ for $\alpha < 1$ OR
- if $f_A < 0$ and $f_I > 0$ for $\alpha > 1$

pe_c followes from (3.13) and is given by:

$$pe_c = \frac{(1+\alpha)(1+4\pi^2 l^2/L^2)}{A_0 f_A + I_0 f_I} \tag{3.15}$$

$f_A > 0$ implies that A up-regulates the active stress and $f_I < 0$ implies that I down-regulates the active stress. So an oscillatory instability occurs when the up-regulator (A) of active stress is fast diffusing compared to the down-regulator (I) of active stress $(\alpha < 1)$ and vice-versa.

These conditions for advection-diffusion systems look very similar to the Turing instability conditions for reaction-diffusion equations, although here, the instability is *'mechano-chemical'* in nature.

For large enough peclet values, it is interesting to note that the oscillatory states are unstable and they transition into stationary states, which can be seen in the phase portrait (figure 3.5).

3.3 Numerical Solution and Analysis

After non-dimensionalizing of the main governing equations, two control parameters remain, they are β and the peclet number $(pe = \frac{Ul}{D})$. These are varied as shown in the phase portrait figure 3.5 to get oscillating states as well as stationary states. MATLAB was used to generate the plots [3].

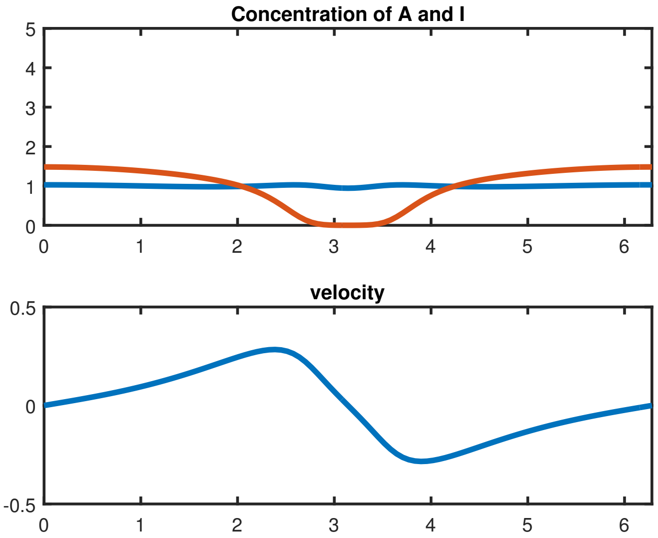

FIGURE 3.1: Oscillatory patterns can be seen. A is represented by the blue line and I by the red line.

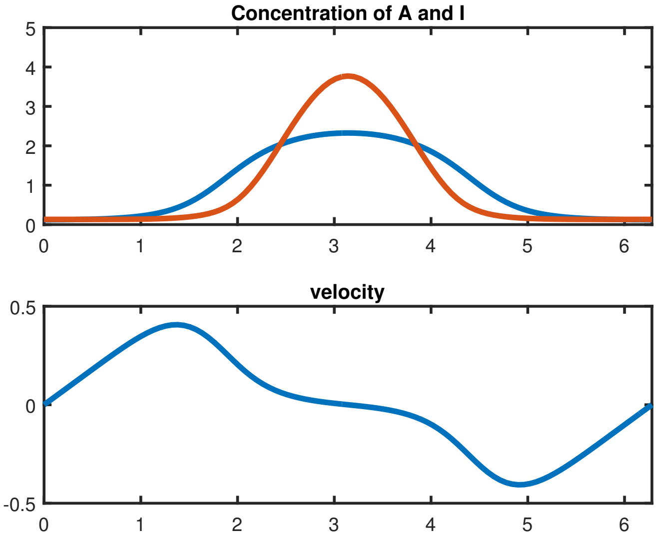

FIGURE 3.2: The concentration peaks can be seen. I is forming a bigger peak than that of A

Consider that A is an up-regulator and I is a down-regulator of active stress, and that I is slower diffusing than A. Now, oscillatory states can be reasoned out as follows:

When the local concentration of I is less as seen in the figure 3.1, then the active stress is higher, and this drives convergent flows. This convergent flow, also brings in both the chemical species A and I and hence both of them peak at a place. As these chemical species have different rates of diffusion, and I being slow, it forms a sharper

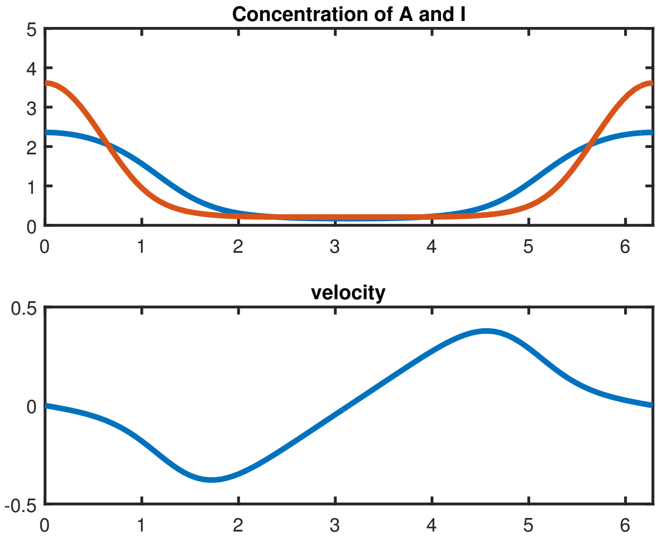

FIGURE 3.3: The peaks are forming at a different place now.(Periodic boundary condition employed). Oscillatory patterns obtained at $\beta = 3.0, pe = 6.5$

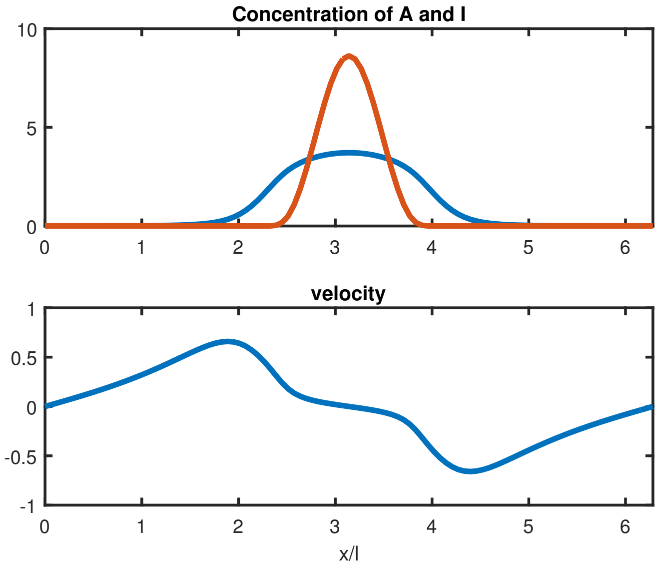

FIGURE 3.4: Stationary patterns obtained at $\beta = 2.5, pe = 7.0$

peak compared to A as seen in figure 3.2. This reduces the convergent flow, and both the peaks of A and I start to relax by diffusion but the peak I remains longer than peak A which intern again enforces divergent flows from the remaining peak I. This process hence makes A and I peak in a different region as seen in the figure 3.3 and the cycle repeats again. If the ratio of advection to diffusion is increased by increasing the peclet number, then oscillatory states transition to stationary states as seen in the figure 3.5.

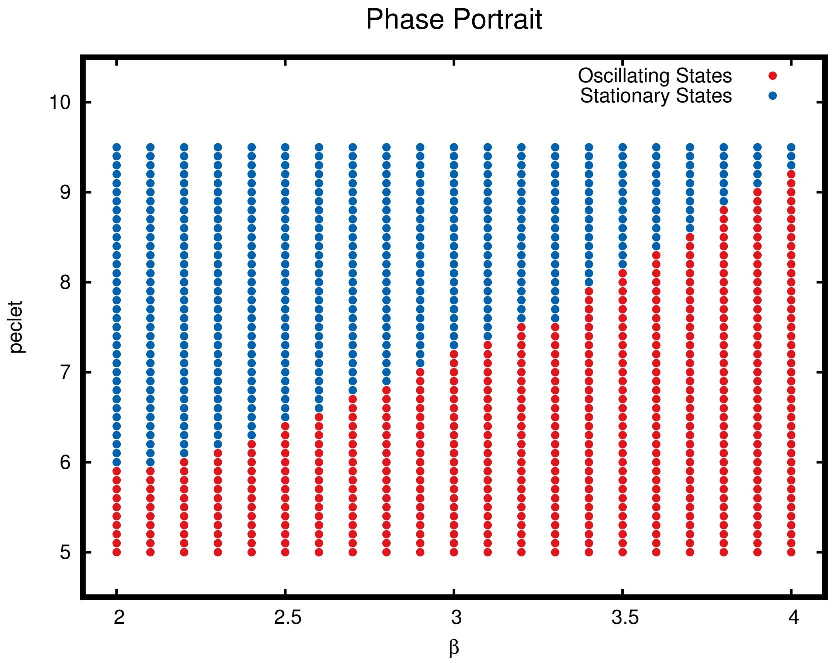

FIGURE 3.5: Phase portrait. It can be seen that if the peclet number is increased for a particular value of β, there is a transition of the numerical solution from oscillatory to stationary states

3.4 Conclusions

It was seen through linear stability analysis that the system of advection-diffusion equations considered here, should give rise to an oscillatory instability and hence oscillations should be observed. This was confirmed by solving the set of these equations numerically and generating video clips of the time series to visualize the oscillations. The conditions obtained for oscillations look very much like the Turing instabilities but these were obtained without involving any chemical reactions. Spontaneous patterns can emerge and oscillate in a system where two diffusing chemical species are considered, much like the Turing system. But the nature of instabilities are mechano-chemical in this context, which is very much different than the chemical instabilities obtained by Turing. The next question of interest would be to see what happens if this system is extended to two dimensions.

References

[1] K. Vijay Kumar, Justin S. Bois, Frank Jlicher and Stephan W. Grill *Phys. Rev. Lett* **112**, 208101 (2014)

[2] L.D. Landau and E.M Lifshitz *Fluid Mechanics* (Second Edition, Pergamon Press, 1987).

[3] Matlab, **R2015a**, (8.5.0.197613), The MathWorks, Inc

Chapter 4

Active Fluid In Higher Dimensions

The previous model of the active fluid, can be extended to higher dimensions. Here we will be looking at a two dimensional model. We will also be looking at multiple chemical species and if patterns can form in such a context. No results have yet been obtained for this framework and this work is still in progress. Nevertheless, a general framework will be presented here.

4.1 Advection Reaction Diffusion Equation

In the previous chapter, it was seen that for oscillations, it was necessary that the two chemical species diffuse at different rates. Here the same thing can be achieved by allowing the two chemical species to have different relaxation times through linear chemical kinetics [1].

Consider two chemical species of concentration A and I [2].

$$\partial_t A = -\nabla \cdot (\mathbf{v}A) + D\nabla^2 A - \kappa(A - A_0) \tag{4.1}$$

$$\partial_t I = -\nabla \cdot (\mathbf{v}I) + D\nabla^2 I - \rho\kappa(I - I_0) \tag{4.2}$$

Here κ is the turnover rate of A. $\rho > 0$ is the ratio of the turn over rate of A to that of I. A_0 and I_0 are the steady state concentrations of the two chemical species, with diffusion coefficient D. The bulk velocity $\mathbf{v}$ can be given by the force balance equation as follows:

$$\nabla \cdot \sigma = \gamma \mathbf{v} \qquad \sigma = \sigma_p + \zeta \Delta\mu \mathbb{I} \tag{4.3}$$

The stress here consists of passive stress σ_p, which comes from the Navier-Stokes equation [3], and the active stress $(\zeta\Delta\mu)_0 f(c)\mathbb{I}$, where $c = (A, I)$ and f is a dimensionless function given by:

$$f(c) = (1+\beta)\frac{A}{1+A} + (1-\beta)\frac{I}{1+I} \tag{4.4}$$

The passive stress is given by:

$$\sigma_p = \eta \left[\nabla \mathbf{v} + (\nabla \mathbf{v})^T - \frac{2}{d}(\nabla \cdot \mathbf{v})\mathbb{I} \right] + \eta_v (\nabla \cdot \mathbf{v})\mathbb{I} \tag{4.5}$$

The passive stress consists terms with shear viscosity (η) as well as bulk viscosity (η_v). d denotes the space dimension

4.1.1 In Two Dimensions

If these equations are explicitly written for a case of 2 space dimensions, they reduce to the following:

Equations (4.1) and (4.2) can be written as

$$\frac{\partial A}{\partial t} = -\frac{\partial v_x A}{\partial x} - \frac{\partial v_y A}{\partial y} + D\frac{\partial^2 A}{\partial x^2} + \frac{\partial^2 A}{\partial y^2} - \kappa(A - A_0) \tag{4.6}$$

$$\frac{\partial A}{\partial t} = -\frac{\partial v_x A}{\partial x} - \frac{\partial v_y A}{\partial y} + D\frac{\partial^2 A}{\partial x^2} + \frac{\partial^2 A}{\partial y^2} - \kappa(A - A_0) \tag{4.7}$$

The equations for velocities will be:

$$\gamma v_x = \eta \left(\frac{\partial^2 v_x}{\partial x^2} + \frac{\partial^2 v_x}{\partial y^2} \right) + \eta_v \left(\frac{\partial^2 v_x}{\partial x^2} + \frac{\partial^2 v_y}{\partial x \partial y} \right) + (\zeta\Delta\mu)_0 \frac{\partial f(c)}{\partial x} \tag{4.8}$$

$$\gamma v_y = \eta \left(\frac{\partial^2 v_y}{\partial x^2} + \frac{\partial^2 v_y}{\partial y^2} \right) + \eta_v \left(\frac{\partial^2 v_y}{\partial y^2} + \frac{\partial^2 v_x}{\partial x \partial y} \right) + (\zeta \Delta\mu)_0 \frac{\partial f(c)}{\partial y} \tag{4.9}$$

These four equations (4.6), (4.7), (4.8), (4.9) are the main governing equations for the dynamics in two dimensions. These equations need to be non-dimensionalized and then numerical results need to be obtained.

4.2 Conclusion

It was seen in chapter 2 that one can get spontaneous patterns to form much like the Turing patterns, even in the absence of reactions, and with just one chemical species moving in one dimensions. This was demonstrated numerically as well as theoretically with the help of the linear stability analysis. In chapter 3, two chemical species were taken moving in one dimension, with one chemical species up-regulating the active stress and one chemical species down-regulating the active stress and spatial oscillations in peaks of these concentrations were shown. This was also demonstrated theoretically with the help of linear stability analysis as well as numerical results obtained which matched the theory. In this chapter, we have seen how to extend this model to higher dimensions, and equations for two dimensions were explicitly stated. We are expecting to get numerical results for this model in two dimensions as well.

References

[1] Thomas Moore, Zoltan Neufeld, Thesis repost*Australian Mathematical Sciences Institute*, February 2014.

[2] K. Vijay Kumar, Justin S. Bois, Frank Jlicher and Stephan W. Grill *Phys. Rev. Lett* **112**, 208101 (2014)

[3] L.D. Landau and E.M Lifshitz *Fluid Mechanics* (Second Edition, Pergamon Press, 1987).

Appendix A

Discretization Procedure

A.1 1-Dimensional system, 1 Diffusing species

The two governing coupled partial differential equations, in the non-dimensionalized form is given below:

$$\frac{\partial c}{\partial T} + pe\frac{\partial (Vc)}{\partial X} = \frac{\partial^2 c}{\partial X^2} \tag{A.1}$$

$$\frac{\partial^2 V}{\partial X^2} + \frac{\partial f(c)}{\partial X} = V \tag{A.2}$$

where $f(c) = \frac{c}{1+c}$, $T = \frac{t}{\tau}$, $X = \frac{x}{l}$. c is the concentration and pe denotes the peclet number

A.1.1 Numerical solution

$$\frac{\partial^2 V}{\partial X^2} = \frac{V_{i+1} - 2V_i + V_{i-1}}{(dX)^2} \tag{A.3}$$

$$\frac{\partial f(c)}{\partial X} = \frac{c_{i+1} - c_{i-1}}{(1 + c_i)^2)(2dX)} \tag{A.4}$$

Substituting (A.3) and (A.4) in (A.2) and rearranging, we get the equation for velocity.

$$V_i = \frac{1}{(2 + (dX)^2)}\left[\frac{(dX)(c_{i+1} - c_{i-1})}{2(1 + c_i^2} + V_{i+1} + V_{i-1}\right] \tag{A.5}$$

Similarly,

$$\frac{\partial c}{\partial T} = \frac{c_i^{t+1} - c_i^t}{dT} \tag{A.6}$$

$$\frac{\partial^2 c}{\partial X^2} = \frac{c_{i+1}^t - 2c_i^t + c_{i-1}^t}{(dX)^2} \tag{A.7}$$

$$\frac{\partial (Vc)}{\partial X} = V_i \frac{(c)_{i+1}^t - (c)_{i-1}^t}{2dX} + c_i \frac{(V)_{i+1}^t - (V)_{i-1}^t}{2dX} \tag{A.8}$$

Substituting (A.6) , (A.7) and (A.8) in (A.1) and rearranging, we get the equation for concentration.

$$c_i^{t+1} = c_i^t + \frac{(dT)(c_{i+1}^t - 2c_i^t + c_{i-1}^t)}{(dX)^2} - (dT)(pe)\left[V_i \frac{(c)_{i+1}^t - (c)_{i-1}^t}{2dX} + c_i \frac{(V)_{i+1}^t - (V)_{i-1}^t}{2dX}\right] \tag{A.9}$$

(here t denotes the index in the time domain and i denotes the index in the space domain)

Equations (A.5) and (A.9) are the ones to be put into the program.

A.1.2 Initial Conditions Used

$c_i = c_0 +$ small perturbation $= 1.0 + 0.00001 sin(x_i)$

$v_i = 0.0$

$x = [0, 2\pi]$ and $i = 1$ to 100

$dX = \frac{2\pi}{100}$ and $dT = \frac{dX}{2000}$

number of time steps run $= 1000000$

A.2 1-Dimensional system, 2 Diffusing Species

The 3 governing coupled partial differential equations in the non-dimensionalized form are given below:

$$\frac{\partial A}{\partial T} + pe\frac{\partial (VA)}{\partial X} = \frac{\partial^2 A}{\partial X^2} \tag{A.10}$$

$$\frac{1}{\alpha}\frac{\partial I}{\partial T} + \frac{pe}{\alpha}\frac{\partial (VI)}{\partial X} = \frac{\partial^2 I}{\partial X^2} \tag{A.11}$$

$$\frac{\partial^2 V}{\partial X^2} + \frac{\partial f(c)}{\partial X} = V \tag{A.12}$$

where $f(c) = \frac{(1+\beta)A}{1+A} + \frac{(1-\beta)I}{1+I}$, $T = \frac{t}{\tau}$, $X = \frac{x}{l}$. A and I are the concentration and pe denotes the peclet number, $\alpha = 0.1$

A.2.1 Numerical solution

$$\frac{\partial A}{\partial T} = \frac{A_i^{t+1} - A_i^t}{dT} \tag{A.13}$$

$$\frac{\partial^2 A}{\partial X^2} = \frac{A_{i+1}^t - 2A_i^t + A_{i-1}^t}{(dX)^2} \tag{A.14}$$

$$\frac{\partial (VA)}{\partial X} = V_i \frac{(A)_{i+1}^t - (A)_{i-1}^t}{2dX} + A_i \frac{(V)_{i+1}^t - (V)_{i-1}^t}{2dX} \tag{A.15}$$

Substituting (A.13), (A.14) and (A.15) in (A.10) and rearranging, we get the equation for concentration of A.

$$A_i^{t+1} = A_i^t + \frac{(dT)(A_{i+1}^t - 2A_i^t + A_{i-1}^t)}{(dX)^2} - \frac{(dT)(pe)}{2dX}\left[V_i^t[(A)_{i+1}^t - (A)_{i-1}^t] + A_i^t[(V)_{i+1}^t - (V)_{i-1}^t]\right] \tag{A.16}$$

Similarly we get equations for concentration of I.

$$I_i^{t+1} = I_i^t + \frac{(\alpha dT)(I_{i+1}^t - 2I_i^t + I_{i-1}^t)}{(dX)^2} - \frac{(dT)(pe)}{2dX}\left[V_i^t[(I)_{i+1}^t - (I)_{i-1}^t] + I_i^t[(V)_{i+1}^t - (V)_{i-1}^t]\right] \tag{A.17}$$

(here 't' denotes the index in the time domain and 'i' denotes the index in the space domain)

Similarly

$$\frac{\partial^2 V}{\partial X^2} = \frac{V_{i+1} - 2V_i + V_{i-1}}{(dX)^2} \tag{A.18}$$

$$\frac{\partial f(c)}{\partial X} = \frac{(1+\beta)(A_{i+1} - A_{i-1})}{2dX(1+A_i)^2} + \frac{(1-\beta)(I_{i+1} - I_{i-1})}{2dX(1+I_i)^2} \tag{A.19}$$

Substituting (A.18) and (A.19) in (A.12) and rearranging, we get the equation for velocity.

$$V_i = \frac{1}{(2+(dX)^2)}\left[\frac{(dX)(1+\beta)(A_{i+1}-A_{i-1})}{2(1+A_i)^2}+\frac{(dX)(1-\beta)(I_{i+1}-I_{i-1})}{2(1+I_i)^2}+V_{i+1}+V_{i-1}\right] \tag{A.20}$$

Equations (A.16) , (A.17) and (A.20) are the ones to be put into the program.