CL-716
Modelling Chemical and Biological Patterns
BIFURCATION ANALYSIS OF NONLINEAR REACTION-DIFFUSION EQUATIONS

Project Presentation

Group 11

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Akash Deep Singhal (11D020024)

Amit Agarwal (11D020014)

Abstract

The theoretical expressions are limited to the neighborhood of the marginal stability point. Computer simulations allow not only the verification of their predictions but also the investigation of the behavior of the system for larger deviations from the instability point.

Introduction

- Chemical Reaction
- Rate Equation
- Boundary Conditions

Chemical Reaction

- The theory of dissipative structures have been illustrated on a simple model system involving the following set of coupled chemical reactions:

$$
\left.\begin{array}{lr}
A \rightleftharpoons X & \text{(a)} \\
2X + Y \rightleftharpoons 3X & \text{(b)} \\
B + X \rightleftharpoons Y + D & \text{(c)} \\
X \rightleftharpoons E & \text{(d)}
\end{array}\right\} \quad (1.1)
$$

- The system is open to the initial and final chemicals A, B, D and E, whose concentrations are imposed throughout the system
- Nonlinearity is introduced by the auto- and cross-catalytic steps (b) and (c);

Rate Equations

- The rate equations of our nonlinear reaction-diffusion system are given by:

$$\frac{\partial X}{\partial t} = A + X^2 Y - (B + 1)X + D_X \cdot \frac{\partial^2 X}{\partial r^2}$$
$$\frac{\partial Y}{\partial t} = BX - X^2 Y + D_Y \cdot \frac{\partial^2 Y}{\partial r^2} \quad (0 \leqslant r \leqslant L). \tag{1.2}$$

Where, D_x and D_y are the diffusion coefficients of X and Y

- Assumption: Fick's law is valid

Boundary Conditions

Two types of boundary conditions will be considered:

1. Zero flux boundary conditions (Neumann conditions):

$$\frac{\partial}{\partial r} X(0, t) = \frac{\partial}{\partial r} X(L, t) = \frac{\partial}{\partial r} Y(0, t) = \frac{\partial}{\partial r} Y(L, t) = 0 \quad (t \geqslant 0). \quad (1.3)$$

2. Fixed boundary conditions (Dirichlet conditions):

$$\begin{aligned} X(0, t) &= X(L, t) = A \\ Y(0, t) &= Y(L, t) = B/A \quad (t \geqslant 0). \end{aligned} \quad (1.4)$$

Matlab Code

- The main script
- PDE Solver
- Initial Condition
- Boundary Conditions

Matlab Code

The main script file

```
function pdex4

m=0; %slab
r=linspace(0,pi,100);
t=linspace(0,200,100);
sol=pdepe(m,@pdex4pde,@pdex4ic,@bc2fn,r,t);
disp(sol);

u1 = sol(:,:,1);
u2 = sol(:,:,2);

figure
surf(r,t,u1)
title('X(r,t)')
xlabel('Distance r')
ylabel('Time t')

figure
surf(r,t,u2)
title('Y(r,t)')
xlabel('Distance r')
ylabel('Time t')
```

Matlab Code

PDE solver

```
function [c,f,s] = pdex4pde(r,t,u,DuDr)

% Diffusion Coefficients
Dy = 1.6*10^(-3);
Dx = 8.0*10^(-3);

% Constants
A = 2;
L = 1;
u1 = u(1);
u2 = u(2);

B = 3.7; %NOT GIVEN | TO BE CHANGED

c = [1; 1];
f = [Dx; Dy] .* DuDr;

% Rate equations describing the phenomenon
s1 = A + u1^2*u2 - (B+1)*u1;
s2 = B*u1 - u1^2*u2;

% Linearized equations for the perturbation x and y
% s1 = (B-1)*u1 + A^2*u2;
% s2 = -B*u1 - A^2*u2;

s = [s1; s2];
```

Matlab Code

Initial Conditions

```
function u0 = pdex4ic(r);

% Constants
A = 2;
B = 3.7; %NOT GIVEN | TO BE CHANGED

c1 = 10;
c2 = 10;
L = 1;

u0 = [A;B/A];
```

Matlab Code

Boundary Conditions

```
function [pl,ql,pr,qr]=bc2fn(xl,ul,xr,ur,t)

% Constants
A = 2;
B = 0.4; %NOT GIVEN | TO BE CHANGED

% Case 1:- Zero Flux Boundary Conditions (Neumann conditions)
pl= [0;0];
ql=[1;1];
pr =[0;0];
qr =[1;1];

% Case 2:- Fixed Boundary Conditions (Dirichlet conditions)
% pl = [A; B/A];
% ql = [0; 0];
% pr = [A; B/A];
% qr = [0; 0];
```

Numerical Analysis

- Simulation using Matlab
- Space-time Plots

Numerical Analysis

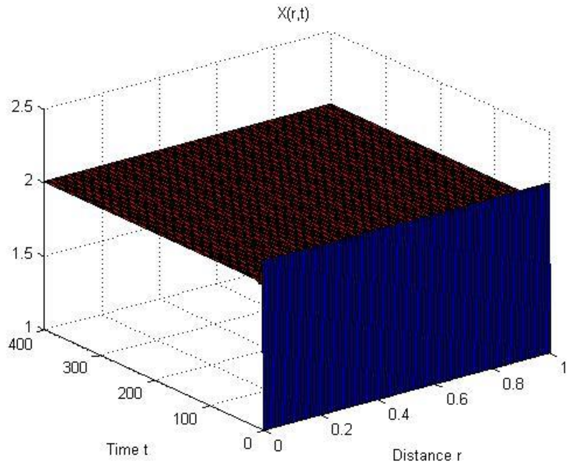
- We use the simulation using MATLAB to verify the numerical results with the analytical ones.

- Following are the major numerical simulations:-

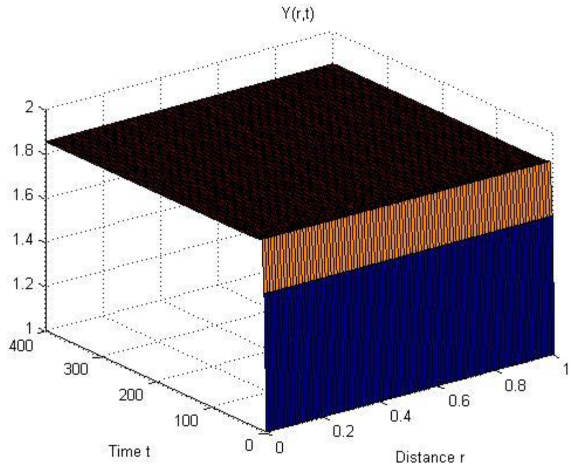
Numerical Analysis

Case 1

- All the equations are restricted to the constraint $0 \leq r \leq L$ and L is taken to be 1.
- Also diffusion coefficients are taken to be:-
  - $Dx = 1.6 \times 10^{-3}$
  - $Dy = 8.0 \times 10^{-3}$
- A = 2 and B = 3.7 for zero flux boundary condition



X vs distance ‘r’ and time ‘t’

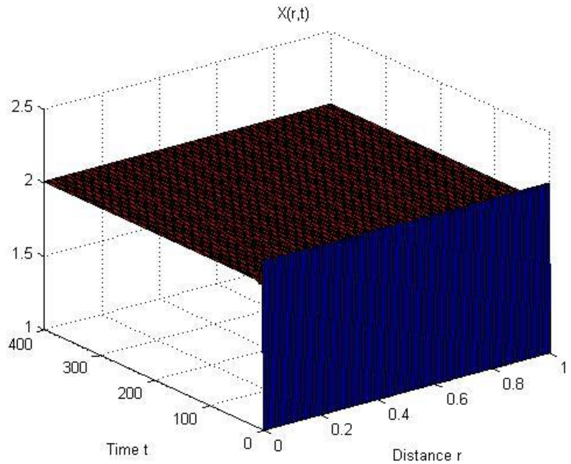


Y vs distance ‘r’ and time ‘t’

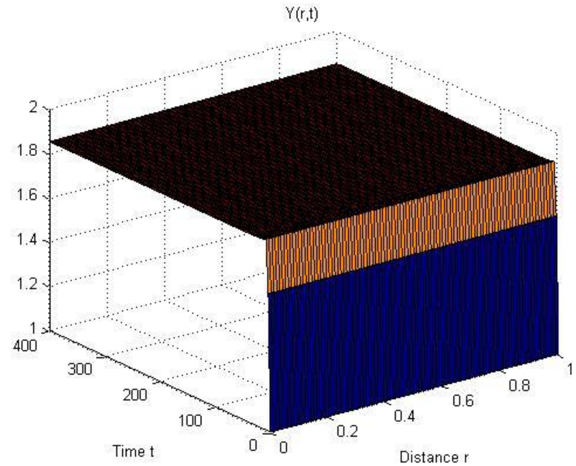
NUMERICAL ANALYSIS

Case 2

- All the equations are restricted to the constraint $0 \le r \le L$ and L is taken to be 1.
- Also diffusion coefficients are taken to be:-
  - $Dx = 8.0 \times 10^{-3}$
  - $Dy = 1.6 \times 10^{-3}$
- A = 2 and B = 3.7 for zero flux boundary condition



X vs distance ‘r’ and time ‘t’



Y vs distance ‘r’ and time ‘t’

Analytical Solution

- General solution
- Linear Stability Diagrams
- Comparison
- Critical Wavenumber

Analytical Solution

- For zero – flux boundary conditions,

$$\begin{pmatrix} x \\ y \end{pmatrix} = \begin{pmatrix} c_1 \\ c_2 \end{pmatrix} e^{w_n t} \cos \frac{n\pi r}{L} \quad (n = 0, 1, 2, 3 \ldots). \tag{2.5b}$$

- Inserting this into the rate equations, we get secular equation relating w_n to the wavenumber n and the system's parameters:

$$w_n^2 - \mathrm{Tr}\, w_n + \Delta = 0 \tag{2.6}$$

where

$$\mathrm{Tr} = B - (A^2 + 1) - \beta(D_X + D_Y)$$

$$\Delta = A^2 + \beta[A^2 D_X + (1 - B)D_Y] + \beta^2 D_X D_Y$$

and

$$\beta = \left(\frac{n\pi}{L}\right)^2.$$

Analytical Solution

- Instability of the thermodynamic branch will occur for some value of n, if at least one of the roots of (2.6) has a positive Re w_n part. The main point is thus to establish the conditions for marginal stability, Re $w_n = 0$, corresponding either to 'exchange of stability', Im $w_n = 0$, or to 'overstability' Im $w_n \neq 0$. A close analysis of (2.6) shows that:

(a) *the values of w_n are complex if:*

$$(A - \delta^{1/2})^2 < B < (A + \delta^{1/2})^2 \tag{2.7}$$

where $\delta = 1 - \beta(D_X - D_Y)$ must be a positive quantity. In this case marginal stability occurs at the critical point:

$$B = B_{1c}(n) = 1 + A^2 + \beta(D_X + D_Y). \tag{2.8}$$

Analytical Solution

- For real w_n's the instability conditions reads:-

$$B \geqslant B(n_c) = \min_{\substack{n \geq 1 \\ \text{integer}}} \left\{ 1 + \frac{D_X}{D_Y} A^2 + \frac{A^2}{D_Y \beta} + \beta D_X \right\} \tag{2.13}$$

Linear stability diagram

Case I

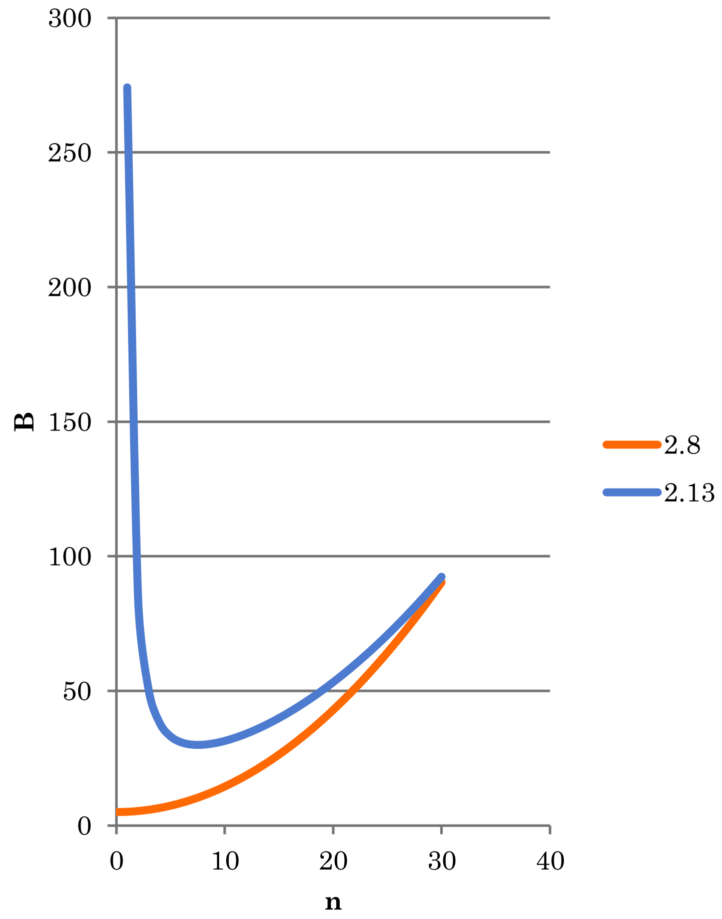
A=2

B=3.7

L=1

Dx = 8.0 x 10^{-3}

Dy = 1.6 x 10^{-3}



Linear stability diagram

Case II

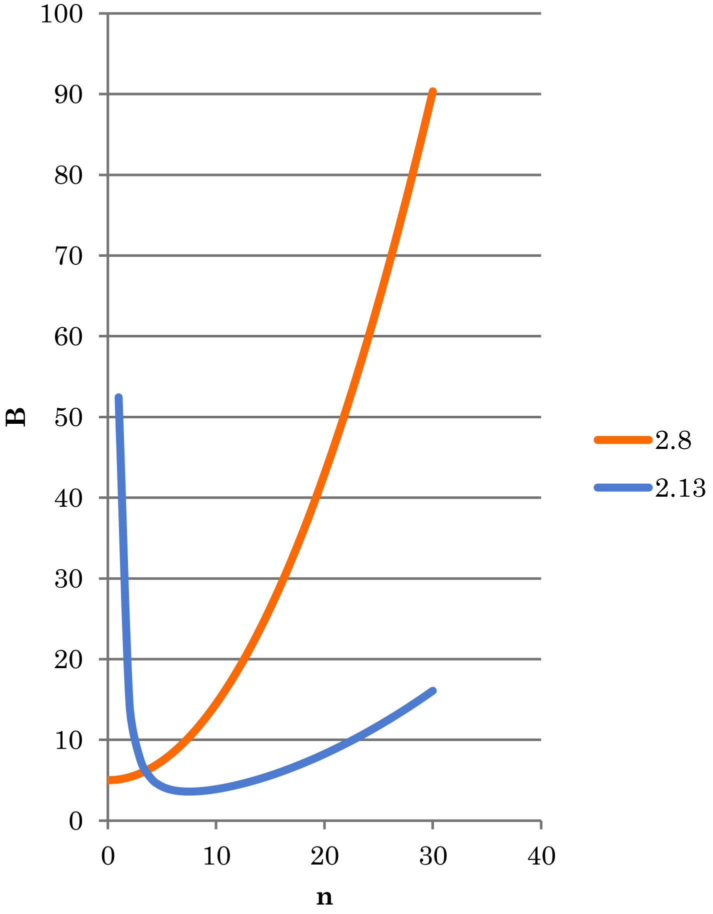
A=2

B=3.7

L=1

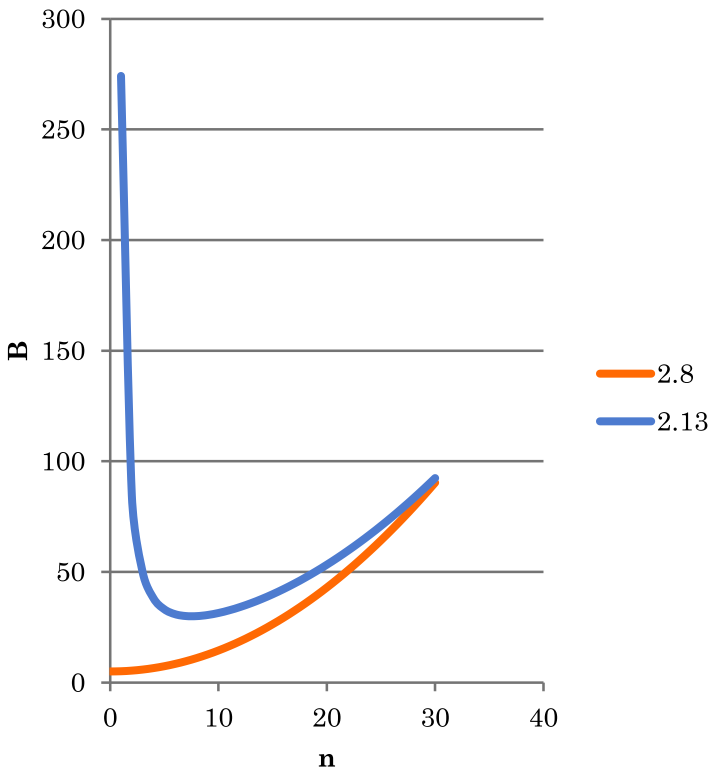
$Dx = 1.6 \times 10^{-3}$

$Dy = 8.0 \times 10^{-3}$

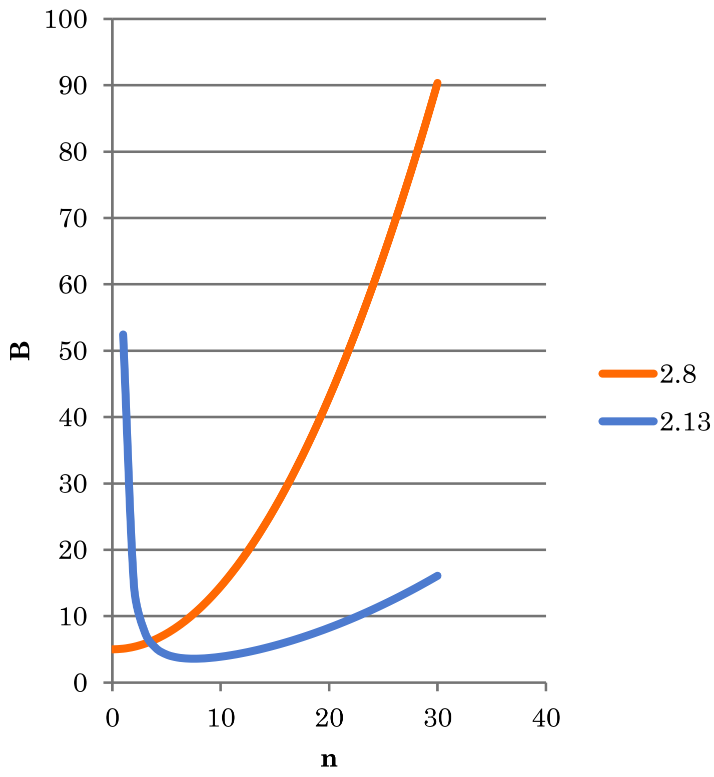


Linear stability diagram: Comparison

Case I

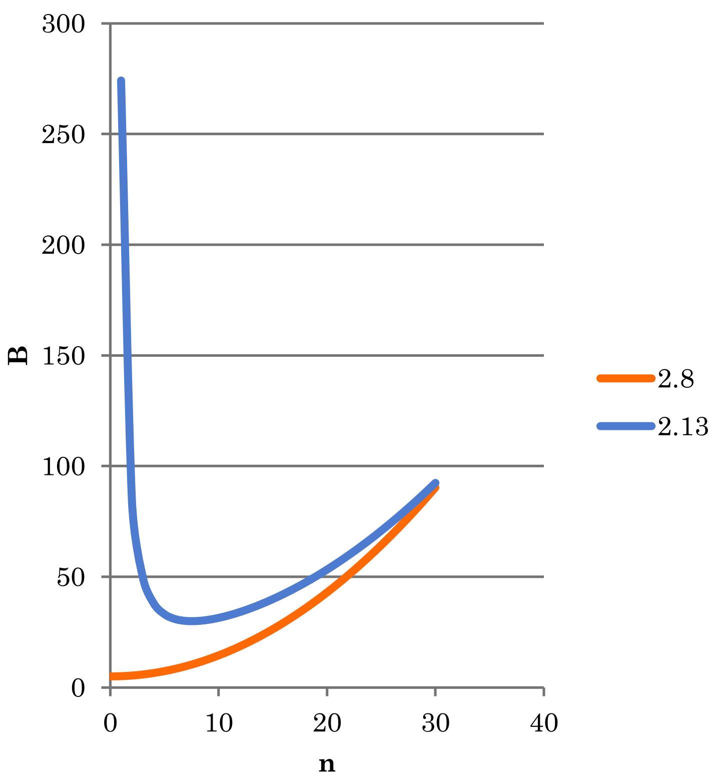


Case II

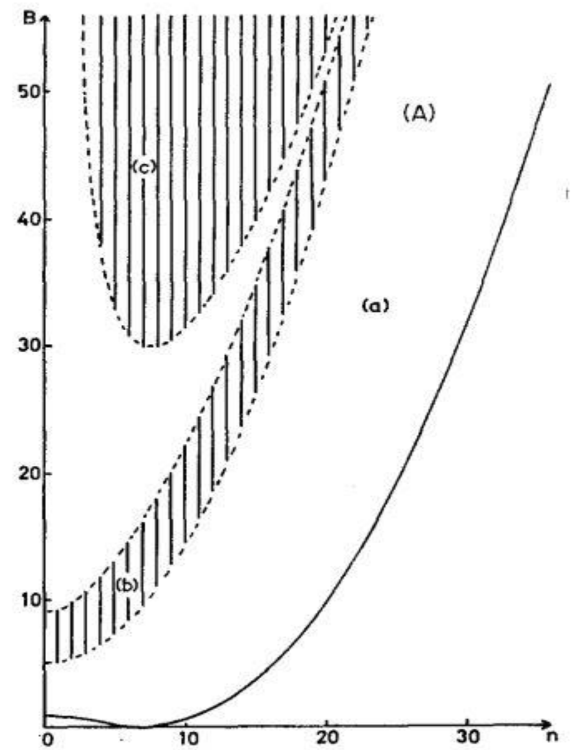


Linear stability diagram: Validity Verification (Case I)

Numerical

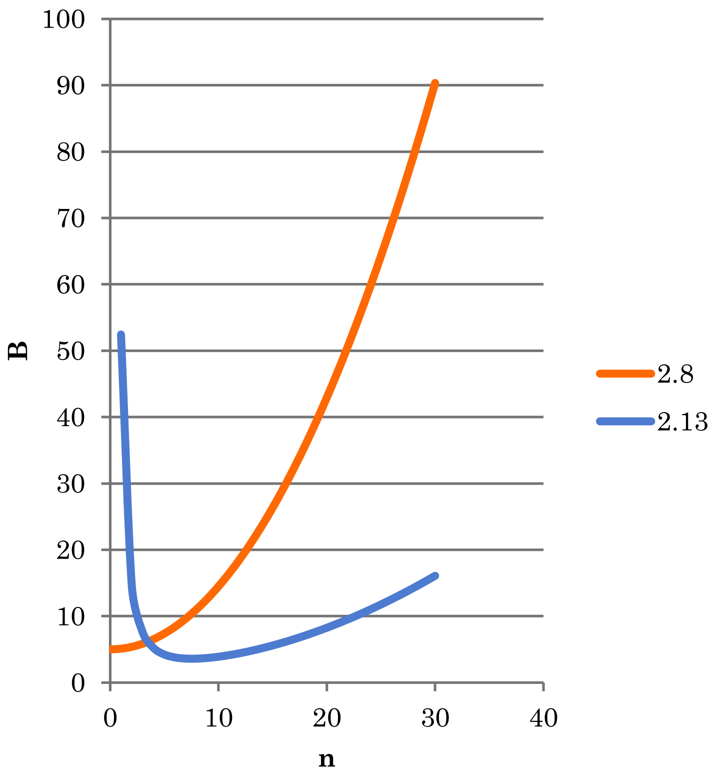


Analytical

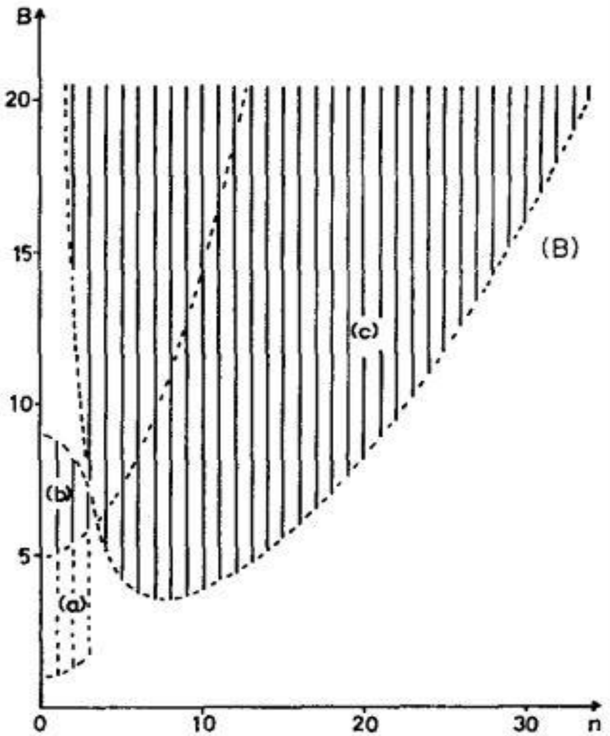


Linear stability diagram: Validity Verification (Case II)

Numerical



Analytical



Critical Wave Number

- The critical wave number corresponding to the onset of stability is given by n_{min} if it is an integer or by one of the two closest integers.

$$n_{\min} = \frac{L}{\pi} \cdot \frac{A^{1/2}}{(D_X D_Y)^{1/4}} \qquad (2.11)$$

Case I: A=2, B=3.7, L=1, Dx = 8.0 x 10^{-3}, Dy = 1.6 x 10^{-3}
Critical Wave number = $[1/\prod * 2^{1/2}/(8*10^{-3}*1.6*10^{-3})^{1/4}] = 8$

Case II: A=2, B=3.7, L=1, Dx = 1.6 x 10^{-3}, Dy = 8.0 x 10^{-3}
Critical Wave number = $[1/\prod * 2^{1/2}/(1.6*10^{-3}*8*10^{-3})^{1/4}] = 8$ (same)

Extended Analysis

- Analytical steady state dissipative structure
- Properties of the Dissipative Structure
- Matlab code

ANALYTICAL STEADY STATE DISSIPATIVE STRUCTURE

- We have,

$$\frac{\gamma_2}{c_1^2} = -\frac{3}{4} \cdot \frac{D_X\beta + 1 - B_c}{A^2} + \frac{1}{A^2}[2(D_X\beta + 1) - B_c]$$
$$-\frac{2}{9} \cdot \frac{[2(D_X\beta + 1) - B_c][\frac{11}{4}D_X\beta + 2 - B_c]}{A^2 D_X\beta} \qquad (2.39)$$
$$= \phi(n_c, A, D_X, B_c).$$

The bifurcating non uniform steady state solution near $B = B_c$ is thus approximated by:

$$x(r) = \pm\left(\frac{B - B_c}{\phi}\right)^{1/2} \cos\frac{n_c\pi r}{L}$$
$$+\frac{2}{9} \cdot \frac{B - B_c}{\phi} \cdot \frac{2(\beta D_X + 1) - B_c}{A D_X\beta} \cos\frac{2n_c\pi r}{L}$$
$$y(r) = \pm\left(\frac{B - B_c}{\phi}\right)^{1/2} \cdot \frac{D_X\beta + 1 - B_c}{A^2} \cdot \cos\frac{n_c\pi r}{L} \qquad (2.41)$$
$$+\frac{2}{9} \cdot \frac{B - B_c}{\phi} \cdot \frac{[2(\beta D_X + 1) - B_c][\frac{7}{4}D_X\beta + 1 - B_c]}{A^3 D_X\beta} \cos\frac{2n_c\pi r}{L}$$
$$-\frac{1}{2} \cdot \frac{B - B_c}{\phi} \cdot \frac{2(\beta D_X + 1) - B_c}{A^3}.$$

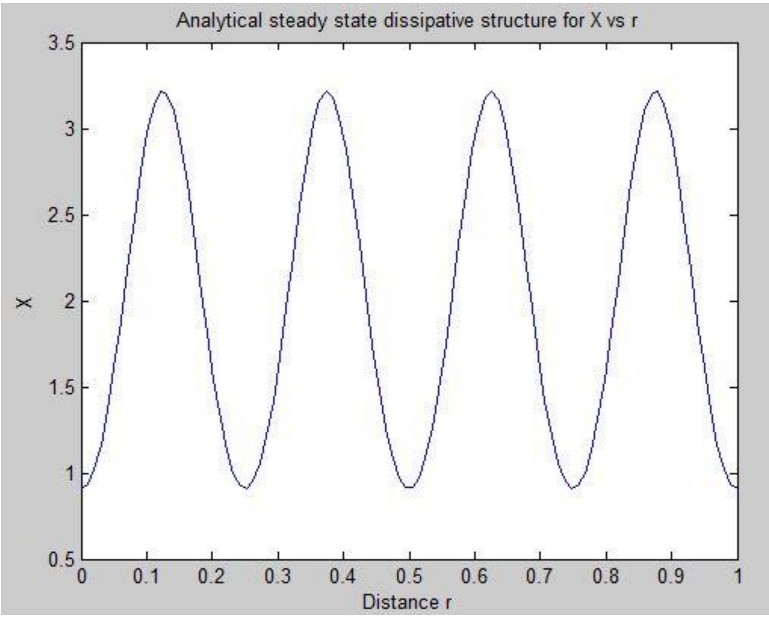
Matlab Code

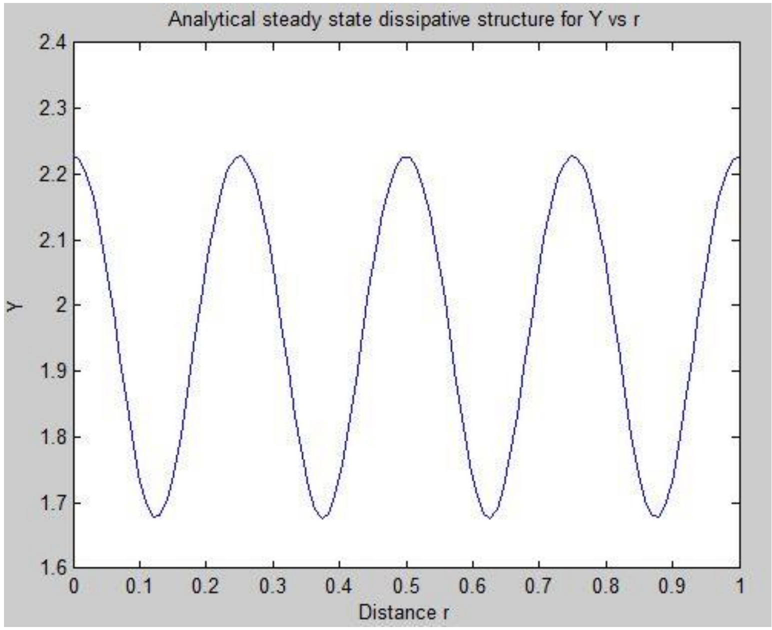
```
A = 2;
B = 4;
Bc = 3.602;

L = 1;
beta = 631.0144;
Dx = 1.6*10^-3;
nc = 8;
fi = -3/4*(beta*Dx + 1-Bc)/(A^2) + 1/A^2*(2*(beta*Dx + 1)-Bc)/(A^2) -
2/9*(2*(beta*Dx + 1)-Bc)*(11/4*Dx*beta+2-Bc)/(A^2*Dx*beta);
r=linspace(0,1,100);

x = -((B-Bc)/fi)^(1/2)*cos(nc*pi*r/L)+2*L+2/9*(((B-Bc)/fi)*(2*(beta*Dx + 1)-
Bc)/(A*Dx*beta))*cos(2*nc*pi*r/L);

y = ((B-Bc)/fi)^(1/2)*(-0.6)*((Dx*beta+1-Bc)/A^2)*cos(nc*pi*r/L) + 2/9*(((B-
Bc)/fi)*(2*(beta*Dx + 1)-Bc)/(A^3*Dx*beta))*((7/4)*Dx*beta + 1 -
Bc)*cos(2*nc*pi*r/L) - (1/2)*((B-Bc)/fi)*(2*(beta*Dx + 1)-Bc)/A^3+2*L;

figure
plot(r,x)
title('Analytical steady state dissipative structure for X vs r')
xlabel('Distance r')
ylabel('X')

figure
plot(r,y)
title('Analytical steady state dissipative structure for Y vs r')
xlabel('Distance r')
ylabel('Y')
```

Dissipative structure pattern

X v/s r

Y v/s r





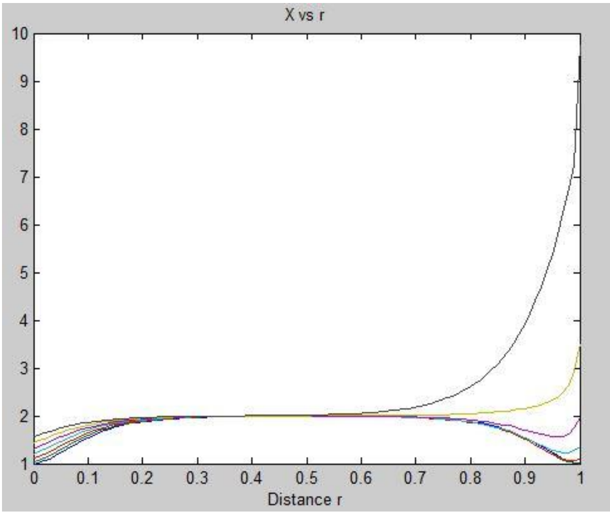
Results obtained from the simulation of the above MATLAB code; Matched with the original solution given in figure 5a and 5b in the paper.

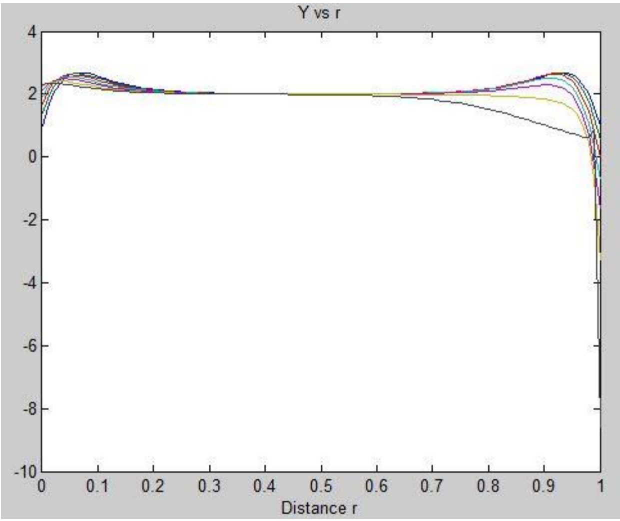
Pattern from numerical integration of steady state rate equation

- And the pattern obtained from numerical integration of equation 1.2,

$$\frac{\partial X}{\partial t} = A + X^2 Y - (B+1)X + D_X \cdot \frac{\partial^2 X}{\partial r^2}$$
$$\frac{\partial Y}{\partial t} = BX - X^2 Y + D_Y \cdot \frac{\partial^2 Y}{\partial r^2} \quad (0 \leqslant r \leqslant L). \tag{1.2}$$

comes out to be as follows:-





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Thank You