TRAVELING WAVE SOLUTIONS OF REACTION-DIFFUSION EQUATIONS COUPLED WITH SHALLOW WATER EQUATIONS

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Abstract

In this thesis, we focus on the existence of a traveling wave solutions for reaction- diffusion equations coupled with shallow water equations. We use the reaction diffusion equations to model the chemical reaction and the diffusion processes of sulfuric acid, which was carried by a barge that capsized into Rhine river in 2011. In most cases, traveling waves solutions of a second order partial differential equation are study by splitting the second order partial differential equation into two first order ordinary differential equations, which may lead to an autonomous system. We show the existence of traveling wave solutions by following the phase plane analysis method and discuss our model in terms of an autonomous system. We develop a numerical scheme based on Finite Volume and Finite Difference method to discretize the Burgers' equation and reaction-diffusion equation respectively. In the implementation, we use MATLAB program to obtain our numerical results.

Keywords: *Traveling wave solution. Chemical Reaction. Diffusion. SWE. Numerical simulation*

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1 Introduction

In the year 2011 [1], a barge carrying 2400 tons of a highly concentrated sulfuric acid capsized on the Rhine river in Germany. Fortunately the barge was provided with a double hall which prevented spill of sulfuric acid. On August 17th, 2005, a barge carrying more than 425,000 gallons of sulfuric acid sits in Chocolate Bayou, Texas [2] and on the 18th August, 1976, a tank barge containing 1060 tonnes of fuming sulfuric acid capsized while being towed across Chesapeake Bay [3]. Within 30 to 60 minutes period, all the cargo on the barge spills in the river, and this lead to a tremendous violent reaction with vast amount of steam and vapor beneath the barge.

From an experimental point of view, the combination of an highly concentrated sulfuric acid and water leads to an unsafe substances in the river and the air around the barge, which it can lead to explosion of the barge. By taking into account the incident that happened on the 18th of August, 1976, where large amount of steam and vapor took place beneath the barge and because of sulfuric acid and water mixture, a violent reaction occurred. Due to this phenomena, we are interested in studying the reaction diffusion processes associated with this type of phenomena using mathematical model.

From the above explanations, we have three cases that we may consider.

1. First case is the air pollutants produced by a chemical reaction
2. Second case is the transfer of the sulfuric acid by a diffusion process
3. And third case is the impacts on living creature inside the river

In our work, we consider only the second case.

We focus on modeling the reaction-diffusion process of the sulfuric acid into the Rhine river. In particular, we use the shallow water equations to describe the movement of the flow in a river. Shallow water equations are a set of hyperbolic partial differential equations that describe the flow of fluid and is also called Saint Venant equations in its one dimensional form, after Adhemar Jean Claude Barre de Saint-Venant [4].The term 'shallow' means that the vertical length is smaller than the horizontal length.

The shallow water equations are derived from the Navier-Stokes equation by integrating it over the water depth, e.g., by integrating the continuity and the momentum equations of the Navier Stokes over the water depth. For more details about the derivation of the shallow water equations, we refer to [5], [6], [7].

In the second part of the model, we study the reaction- diffusion equation which describe the chemical reaction between the sulfuric acid and the water.

The reaction- diffusion equation is a well known model, e.g., in mathematical biology to model the chemotaxis or the population density of bacterias (see [6, 8, 9, 10, 11]). In the chemotaxis model the traveling wave solutions of the reaction diffusion equation bases on the singularity in the logistic term or the nonlinear degenerate term of the cell densities, for more about the chemotaxis model see [11]. In [6] it has been shown that even without a singularity we can ensure a traveling wave solution by introducing a microscopic term in the macroscopic model.

A classical way to investigate traveling wave solutions of second order partial differential equations done by transforming the second order PDEs to a second order ordinary differential equations using the traveling wave Ansatz. Then we split the second odes into two ordinary differential equations representing an autonomous system. We first compute the equilibrium points of the autonomous system, which it corresponds to the steady states of the system, and to determine the stability of the steady states we linerize the set of the equations at these steady states and determine the eigenvalues of the Jacobian matrix. For example in the Fisher equation, has a traveling wave solutions if and only if $s > 2$ while s is the propagation wave speed for more about Fisher equation we refer to [12],[13], [14].

By using the phase plane analysis , we show the existence of a traveling wave solutions to our model in Section 3 and investigate it by the numerical simulation.

The rest of the thesis is organized as follows: In Section 2 we define the mathematical model of our phenomenon and present the simplification and the scaling procedure to our mathematical model. Traveling wave solutions of our mathematical model (8)- (9) are discussed in Section 3. In Section 4 we describe the Finite Volume and Finite Difference methods used to perform a numerical simulation for the system (4),(5). At the end we conclude the main results we obtain from both the analytical method and the numerical simulation with a future scope in Section 5.

2 Mathematical Modeling

2.1 General Model

The general mathematical model that describes the reaction- diffusion process and water flow in a river are defined as

$$\partial_t(h) + \partial_x(hu) = 0 \tag{1}$$

$$\partial_t(hu) + \partial_x(hu^2 + \frac{gh^2}{2}) = -ghH_x \tag{2}$$

$$\partial_t c + u\partial_x c = \partial_x(Dp(u)\partial_x c) + \beta c(1 - \frac{c}{c_\infty}) \tag{3}$$

where

$$\partial_t = \frac{\partial}{\partial t}, \quad \partial_x = \frac{\partial}{\partial x}.$$

The problem we introduced in our introduction gives us the following:

1. The flow of water in the river.
2. Diffusion process of the sulfuric acid in a short period of time in the river.
3. Chemical reaction between the sulfuric acid and the water in the river.

We use the shallow water equations (1),(2) to model the flow of water inside the river, where $u[m.s^{-1}]$ represents the water velocity, $h[m]$ represents the height of water, and both of them depend on space $x[m]$ and time $t[s]$.

For the second point and the third point, we use the reaction diffusion equation (3) to model the reaction and diffusion process of our physical problem.

In equation (3), c $[mole.liter^{-1}]$ represents the concentration of the sulfuric acid inside the river and it depends on space $x[m]$ and time $t[s]$.

In the model (1)-(3) $g[m.s^{-2}]$ is the gravity constant and $H[m]$ is a given function, which describes the bottom topography of the river. D is a constant of dimensional $t[s]$ and $p(u)$ is a given function where $Dp(u)$ represents a dependent diffusion coefficient. $\beta\ [s^{-1}]$ is a constant which represents the chemical reaction time rate, and $c_\infty\ [mole/liter]$ is the maximum value of sulfuric acid concentration per liter, which equals to $19[mole.liter^{-1}]$ or 1890 $[gm.liter^{-1}]$.

In our work, we will not consider the general model (1)-(3), instead we consider a more simple model, which we describe in the next subsections.

2.2 Simplification of the general model

The simplification of the general model (1-3) depend on two main steps.

1. Due to the diffusion process of the sulfuric acid in a short period of time, sedimentation process in the river can be ignored. From this point we can consider the case with zero bed-load which means that the bottom topography of the river is flat.

2. We assume that the water height h is constant, which it follows from the above point.

For the general model of shallow water equation taking into account the sedimentation process we refer to [15],[16].

We summarize the method of how to simplified the general model (1)-(3) as follows:

- We assume that the water height or depth h is constant.

- We consider the case with a zero bed-load.

Equation (1) in the general model can be eliminated by using h as a constant.

By considering the case with zero bed-load where H equals to 0 in the equation (2), leads to our simplified model:

$$\partial_t u + \partial_x(\frac{u^2}{2}) = 0 \tag{4}$$

$$\partial_t c + u\partial_x c = \partial_x(Dp(u)\partial_x c) + \beta c(1 - \frac{c}{c_\infty}) \tag{5}$$

The model equations (4), (5) are the simplified equations of our general model defined in (1)-(3). From the simplified model one observes that the shallow water equations reduced to a first order partial differential equation called inviscid Burgers' equation (4) coupled with the reaction diffusion equation (5).

Burgers' equation is well known model in the context of partial differential equations and it is a wide range model used in physics see [17] .

Now we have a system of partial differential equations in one dimensional form (1-D). Equation (4) describes the velocity flow profile of the water instead of the full shallow water equations in the general model and equation (5) describes reaction-diffusion process of the sulfuric acid.

The model (4),(5) is governed by initial and boundary conditions and these conditions are included in the numerical simulation part in Section 4.

2.3 Scaling the mathematical model

We perform more simplifications to our model (4),(5) by scaling the physical quantities $u(x,t)$ and $c(x,t)$. First we consider the (chemical) concentration of sulfuric acid $c(x,t)$ and the maximum concentration value of the sulfuric acid is ≈ 19 mole per liter or ≈ 1890 gramme per liter. By using the maximum concentration value as a reference, we scale the concentration of the sulfuric acid c to take the value between 0 and 1.

We scale our model (4),(5) by using the scaled quantities which define in Table 2.3 and Table 2.3. Then we get our model (4),(5) in non- dimensional form or a dimensionless form as it is shown from equations (6) and (7).

Unscaled Quantity	Scaled Quantity
x	$x_r\tilde{x}$
t	$t_r\tilde{t}$
u	$u_r\tilde{u}$
c	$c_r\tilde{c}$

Table 1: Scaling quantities

References	Given Values
x_r	100 [m]
t_r	$\frac{1}{\beta}$ [s]
β	0.1 $[s^{-1}]$
u_r	$x_r\beta$ $[\frac{m}{s}]$
c_∞	19 $[\frac{mole}{liter}]$
c_r	c_∞
D	$0.1[s]$

Table 2: References values

$$\partial_{\tilde{t}}\tilde{u} + \partial_{\tilde{x}}(\frac{\tilde{u}^2}{2}) = 0 \tag{6}$$

$$\partial_{\tilde{t}}\tilde{c} + \tilde{u}\partial_{\tilde{x}}\tilde{c} = \lambda\partial_{\tilde{x}}(p(\tilde{u})\partial_{\tilde{x}}\tilde{c}) + \tilde{c}(1-\tilde{c}) \tag{7}$$

where

$$\lambda = D * \beta$$

For convenience, we drop out the tilde and write down the scaled model (6),(7) as follows:

$$\partial_t u + \partial_x(\frac{u^2}{2}) = 0 \tag{8}$$

$$\partial_t c + u\partial_x c = \lambda\partial_x(p(u)\partial_x c) + c(1-c) \tag{9}$$

Equations (8),(9) are written in the dimensionless form and they represent our desired model for the reaction- diffusion process of the sulfuric acid and the flow of water in the river.

Now we want to investigate the existence of traveling wave solutions for the model (8),(9). It follows from Section3.

3 Traveling wave solutions

Think about the wave in the sea, Ocean, or in the river. It can be estimated as a bounded (i.e.finite) ridge of water which moves without changing of its shape.
This estimation forms the basis for the mathematical idea of the traveling wave which can be expressed as a traveling wave ansatz in the form $v(x,t)$ where

$$v(x,t) \equiv v(\xi), \quad \xi = x \pm st, \quad \xi \in R$$

where s is the propagation wave speed and ξ is the traveling wave variable. Traveling wave coordinates is a good procedure to convert the partial differential equations into an ordinary differential equations by combining two independent variables to one independent variable which is called traveling wave variable ξ.
Now we focus on finding positive traveling wave solutions, that is positive solutions of the form $c(x,t) = C(x - st)$, $u(x,t) = U(x - st)$ for some $s > 0$ in the reaction diffusion equation (9) and the Burgers' equation (8) respectively . Here s is the propagation speed of the wave. In addition, it is required that the wave front $C(\xi)$ and the shock wave $U(\xi)$ are defined in $]-\infty, +\infty[$ and satisfies $C(-\infty) = 1$, $C(+\infty) = 0$ and $U(-\infty) = U_l, U(+\infty) = U_r$. This means that we are looking for the solutions of the ordinary differential equations (15)& (16) satisfying the limit conditions (18) .
The equation (15) delivers a shock wave profile, which propagates with a constant speed $s = \frac{U_l+U_r}{2}$ according to Rankine Hugoniot condition see [17]. In [18], it has been shown that the viscid Burgers' equation has a traveling wave solutions and the solutions converges to the solutions of the inviscid burger solution when the viscosity term tends to zero.
Now we apply the phase plan analysis technique. First of all we start by introducing the traveling wave coordinates as follows:

- First we define the traveling wave variable ξ as

$$\xi = x - st$$

with $\xi \in R$, and $s > 0$ is the traveling wave speed or the propagation speed of the wave.

- Second we define the traveling wave Ansatz for both velocity $u(x,t)$ and concentration $c(x,t)$ functions in the following forms

$$U(\xi) = U(x - st) = u(x,t),$$

$$C(x - st) = C(\xi) = c(x,t)$$

.

Using the traveling wave ansatz we have:

$$\partial_t u = -s\frac{dU}{d\xi} = -sU' \tag{10}$$

$$\partial_x u = \frac{dU}{d\xi} = U' \tag{11}$$

$$\partial_t c = -s\frac{dC}{d\xi} = -sC' \tag{12}$$

$$\partial_x c = \frac{dC}{d\xi} = C' \tag{13}$$

$$\partial_{xx} c = \frac{d^2C}{d\xi^2} = C'' \tag{14}$$

Then by substitution of equations (10), (11), (12), (13), (14) in the model (8),(9) we get:

$$-sU' + UU' = 0 \tag{15}$$

$$-sC' + UC' = \lambda(p(U)C')' + C(1 - C) \tag{16}$$

The equations (15),(16) are written in a traveling wave coordinates and they are completed with the following end points conditions

$$U(-\infty) = U_l \quad \text{and} \quad U(+\infty) = U_r \tag{17}$$

$$C(-\infty) = 1 \quad \text{and} \quad C(+\infty) = 0 \tag{18}$$

$$(U_l, U_r) > 0$$

From the boundary conditions (17) of the Burgers' equation, we have two possibilities:

- $U_l < U_r$, in this case we have a rarefaction wave.
- $U_l > U_r$, in this case we have a shock wave profile and it propagates with speed s which equals to the shock wave speed computed by the Rankine Hugoniot condition see [17].

We shall focus on the second case, which means that we have a shock wave profile propagates with the speed s. Here the shock wave equivalents to a traveling wave solution.

By considering the case when $U_l > U_r$ we expect that $U(\xi)$ will satisfy $U_r < U < U_l$ for all $\xi \in R$ and s is the propagation wave speed or the shock speed .

Now we consider the full model (15), (16) while equation (16) appears to be more complicated, a non-linearity term represents the the chemical reaction process and a diffusion coefficient dependent on u that are describing the reaction diffusion process of the sulfuric acid.

The classical procedure to understand the solution of second order ordinary differential equation is to write the equation in terms of a first order system and to perform a phase plane analysis, in particular if the system turns out to be an autonomous.

We start by considering the Fisher equation (19) as a simple case in order to show the phase plane analysis technique and how we can apply to our model. We start by the Fisher equation

$$C'' + sC' + g(C) = 0 \tag{19}$$

By taking

$$W = C'$$

we get:

$$C' = W \tag{20}$$

$$W' = -sW - g(C) \tag{21}$$

If we set $g(C) = C(1 - C)$ we get:

$$\begin{aligned} C' &= W \\ W' &= -sW - C(1 - C) \end{aligned} \tag{22}$$

The system (22) is an autonomous system of the Fisher equation with two equilibrium points according to the steady states $(C', W') = 0$.

Next, we want to compute the Jacobian matrix of the system (22) which follows from the following equation:

$$J(C, W) = \begin{pmatrix} \frac{\partial f_1}{\partial C} & \frac{\partial f_1}{\partial W} \\ & \\ \frac{\partial f_2}{\partial C} & \frac{\partial f_2}{\partial W} \end{pmatrix} = \begin{pmatrix} 0 & 1 \\ -1 + 2C & -s \end{pmatrix} \tag{23}$$

where

$$f_1 = W,$$

$$f_2 = -sW - C(1 - C).$$

From equation (22) which represents an autonomous system, we compute the equilibrium points at the steady states $C' = W' = 0$, this gives two equilibrium points $(C, W) = (0, 0)$ and $(C, W) = (1, 0)$.

In order to specify the nature of the equilibrium points of the system (22), we determine the eigenvalues of the Jacobian matrix which obtain from the next equation

$$|J - \lambda I| = 0 \tag{24}$$

$$\left| \begin{pmatrix} -\lambda & 1 \\ \\ -1+2C & -s-\lambda \end{pmatrix} \right| = 0 \tag{25}$$

From equation (34) we get:

$$\lambda^2 + s\lambda + (1-2C) = 0 \tag{26}$$

For the equilibrium point $(C, W) = (0, 0)$, we get

$$\lambda_{1,2} = -\frac{s}{2} \pm \frac{1}{2}\sqrt{s^2-4} \tag{27}$$

if $s^2 \geq 4$, the equilibrium point $(0, 0)$ is a stable node and if $s^2 < 4$ $(0, 0)$ is a stable spiral. For the equilibrium point $(C, W) = (1, 0)$, we get

$$\lambda_{1,2} = -\frac{s}{2} \pm \frac{1}{2}\sqrt{s^2+4} \tag{28}$$

then the equilibrium point $(1, 0)$ is a saddle point. The phase plane trajectories determines by the following equation

$$\frac{dW}{dC} = \frac{-CW - C(1-C)}{W} \tag{29}$$

Figure 1 shows the phase plane trajectories of the Fisher equation, the stable node $(0, 0)$ acts as an attractor when $s > 2$.

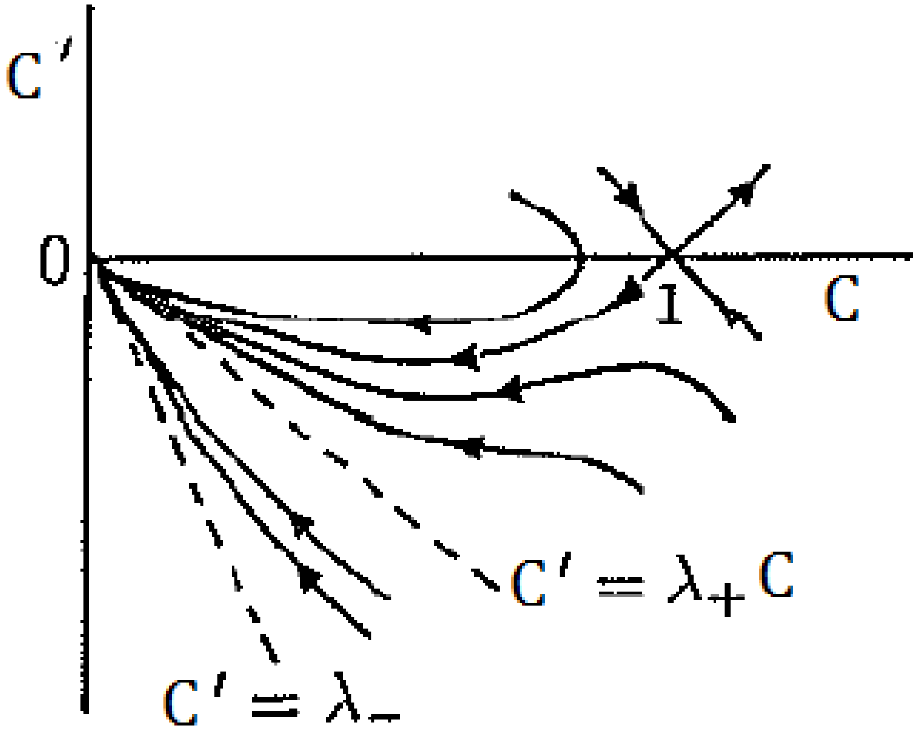

Figure 1: Phase plane trajectories of the Fisher equation [12]

Figure 2 shows the traveling wave front for the Fisher equation. Since C assume negative values if there is a stable spiral at $(C, W) = (0, 0)$, we require $s \geq 2$ for more physical realistic traveling wave solutions. Further more for the traveling wave solutions of the Fisher equation to exist, we require one stable node and one saddle node.

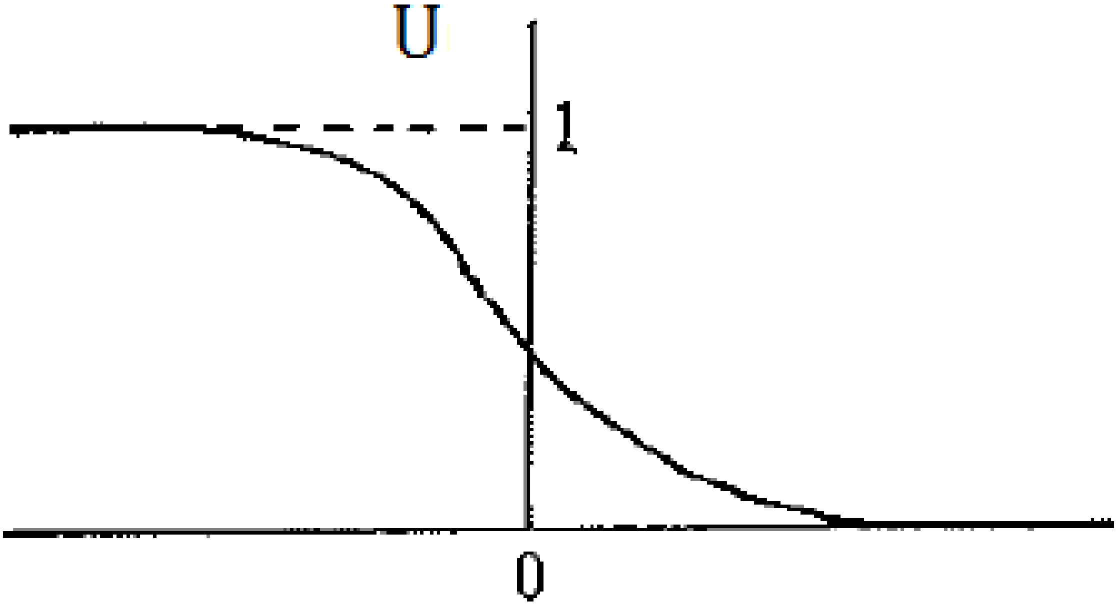

Figure 2: Traveling wave front for C [12]

It has been shown in [19] that for $g \in C^1[0,1]$, there exists a heteroclinc orbit that connecting the equilibrium points $(0,0)$ and $(1,0)$ if and only if $s > s^*$ where $s^* = 2$ see Figure 3 and Figure 4.

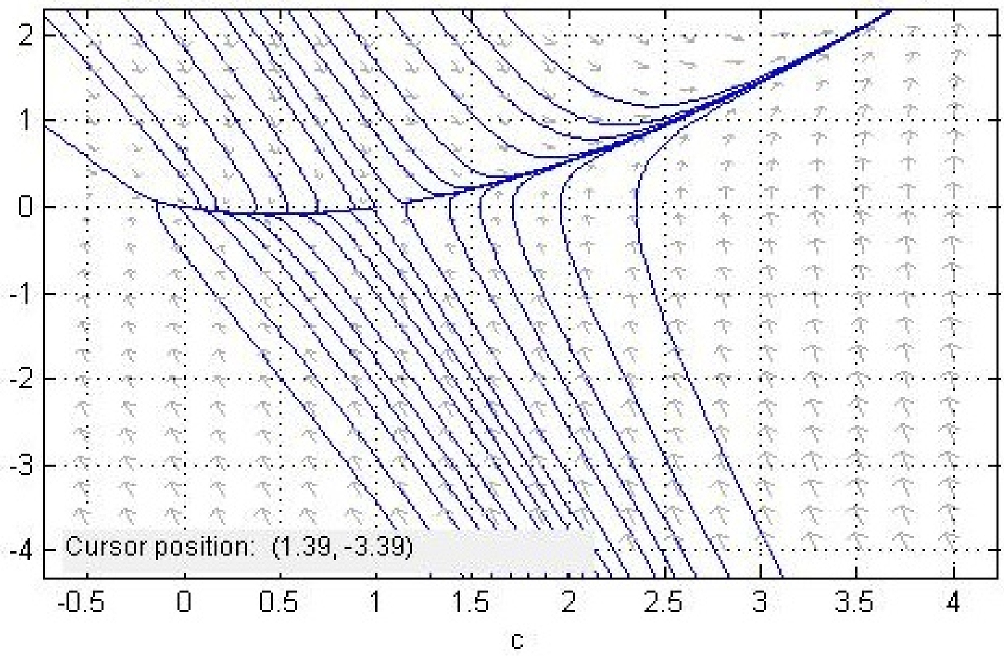

Figure 3: Stable node

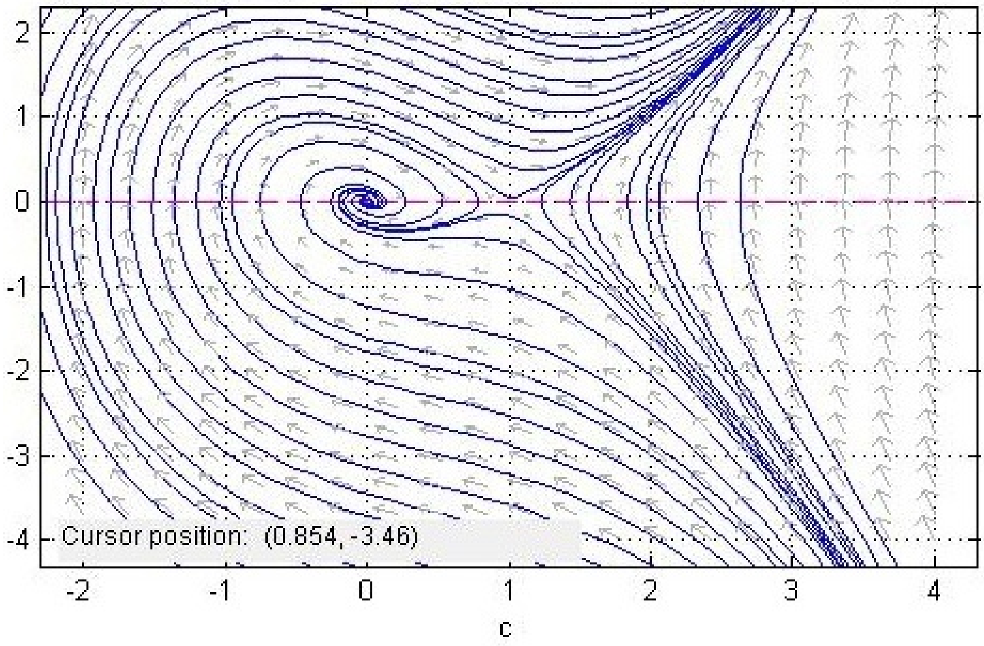

Figure 4: Spiral focus

Now we look at our model (15), (16) and perform the same steps as for the Fisher equation.
From equation (16) we have

$$\lambda p(U)C'' = (-s + U - \lambda p'(U))C' - C(1 - C) \tag{30}$$

We start by writing the equation (15),(30) in terms of a system of differential equations as follows:

$$\begin{aligned} U' &= 0 && (31)\\ C' &= W && (32)\\ W' &= \frac{1}{\lambda p(U)}(U - s - \lambda p'(U))W - \frac{1}{\lambda p(U)}C(1 - C) && (33) \end{aligned}$$

Equations (30), (31), (32) represent an autonomous system. By taking $(U', C', W') = 0$ we compute the equilibrium points of the steady states of the system. We have $(U, 0, 0)$ and $(U, 1, 0)$ as an equilibrium points for all possible values of U. In order to ensure the traveling wave solution to be exist we require one stable node and one saddle point.
First we take the case when $U = 0$ and perform the phase plane analysis, and later on we generalize it for all values of U. We start by linearized the set of equations (30), (31), (32) at the steady states, determine the Jacobian matrix, and determine the eigenvalues of the Jacobian matrix.
The Jacobian matrix reads

$$\text{J(U,C,W)=} \begin{pmatrix} \frac{\partial f_1}{\partial U} & \frac{\partial f_1}{\partial C} & \frac{\partial f_1}{\partial W} \\ \frac{\partial f_2}{\partial U} & \frac{\partial f_2}{\partial C} & \frac{\partial f_2}{\partial W} \\ \frac{\partial f_3}{\partial U} & \frac{\partial f_2}{\partial C} & \frac{\partial f_2}{\partial W} \end{pmatrix} = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & -\frac{1-2C}{p(U)} & \frac{U-s-\lambda p'(U)}{\lambda p(U)} \end{pmatrix}$$

where

$$f_1 = 0,$$

$$f_2 = W,$$

$$f_3 = \frac{1}{\lambda p(U)}(U - s - \lambda p'(U))W - \frac{1}{\lambda p(U)}C(1 - C)$$

Determine the eigenvalues μ of the Jacobian matrix

$$|J - \mu I| = 0 \tag{34}$$

we get

$$\mu[-\mu(\frac{U - s - \lambda p'(U)}{\lambda p(U)} - \mu) + \frac{1 - 2C}{\lambda p(U)}] = 0 \tag{35}$$

We set $p(U)$ to be $(1 + U^2)$ to avoid the case $P(0) = 0$ and we have $\delta = \frac{1}{\lambda}$ such that $\lambda = D * \beta$.

For the equilibrium point $(0, 0, 0)$ we have the following eigenvalues μ:

$$\mu_1 = 0,$$

$$\mu_{2,3} = \frac{\delta}{2}(-s \pm \sqrt{s^2 - \frac{4}{\delta}})$$

then the origin $(0, 0, 0)$ is a stable node if

$$s^2 \geq \frac{4}{\delta}$$

and a stable spiral if

$$s^2 < \frac{4}{\delta}.$$

For the second equilibrium point $(0, 1, 0)$ we have the following eigenvalues μ:

$$\mu_1 = 0,$$

$$\mu_{2,3} = \frac{\delta}{2}(-s \pm \sqrt{s^2 + \frac{4}{\delta}})$$

then the point $(0, 1, 0)$ is a saddle point. We can conclude that for the propagation wave speed $s \geq (2/\sqrt{\delta})$ we have one stable node and one saddle point which ensures the traveling wave solution to exist.

Now we want to ensure the traveling wave solutions of our system (30), (31), (32) for all possible values of U, this gives a large number of equilibrium points at the steady states. During this large amount of equilibrium points it would be difficult to sketch the phase portrait of the set of equations in 3-D, but we are able to estimate a condition for the existence of the traveling wave solutions, which ensures one stable node and one saddle point for every U.

By computing the eigenvalues we get:

$$\mu_1 = 0,$$

$$\mu_{2,3} = \frac{\delta}{2p(U)}(U - s \pm \sqrt{(U-s)^2 - \frac{4p(U)}{\delta}})$$

which correspond to the equilibrium points $(U, 0, 0)$ for all possible value of U and these equilibrium points are either a stable node if

$$(U - s) \geq \pm 2\sqrt{p(U)/\delta}$$

or a stable spiral if

$$(U - s) < \pm 2\sqrt{p(U)/\delta}.$$

Furthermore, we have the eigenvalues

$$\mu_1 = 0,$$

$$\mu_{2,3} = \frac{\delta}{2p(U)}(U - s \pm \sqrt{(U-s)^2 + \frac{4p(U)}{\delta}})$$

which correspond to the equilibrium points $(U, 1, 0)$ for all possible values of U and these equilibrium points are a saddle point.

We claim that we have more than one stable node and saddle point which are necessary to the existence of a traveling wave solutions of our model with a propagation wave speed

$$(U - s) \geq \pm 2\sqrt{p(U)/\delta}$$

and indeed there exists a heteroclinic orbits connecting the equilibrium points of the system in the steady states due to the fact that the origin $(0, 0, 0)$ acts as an attractor.

One can say that there exists a heteroclinic orbits connecting the equilibrium points of the system if and only if the propagation wave speed satisfies

$$(U - s) \geq \pm 2\sqrt{p(U)/\delta}.$$

We verify the above inequality which grantee the existence of a traveling wave solution in behalf of our numerical simulation in Section 4 by considering the shock wave of the velocity U in Figure 5 and the wave front of the concentration C in Figure 6.

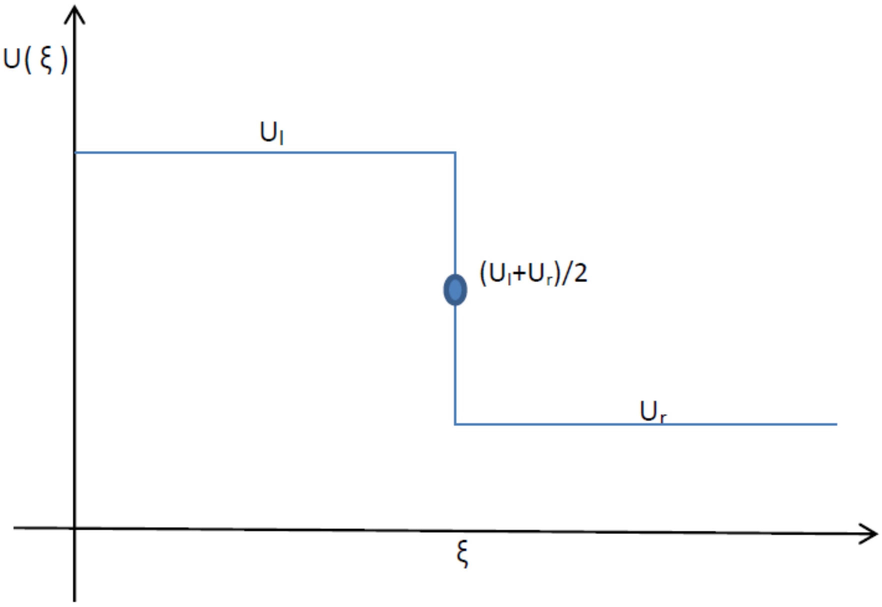

Figure 5: Shock wave front for $U(\xi)$

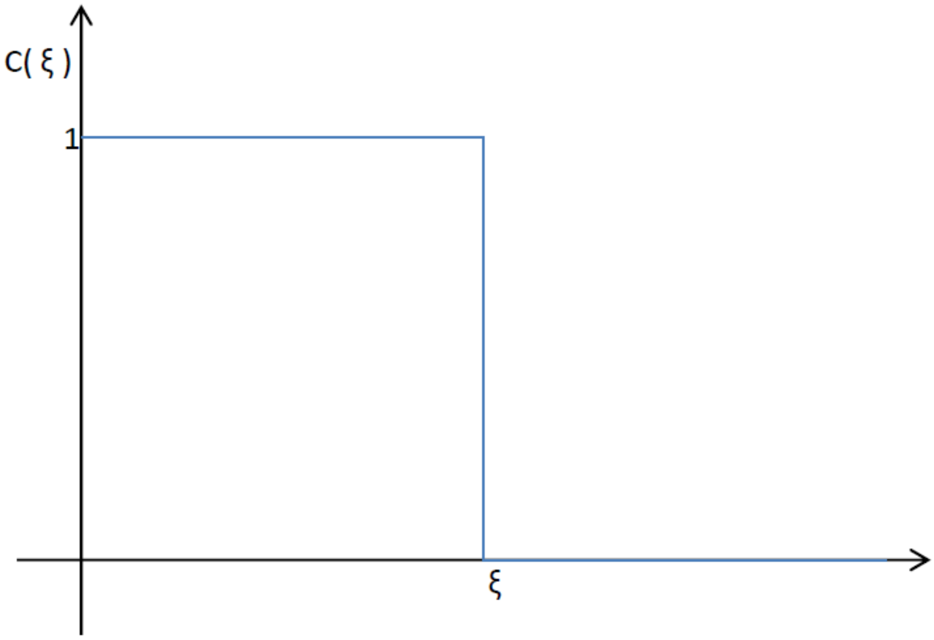

Figure 6: Wave front for $C(\xi)$

Then we expect that the point $(U_r, 0)$ is a stable node if

$$(U - s)^2 > 4\frac{p(U)}{\delta}$$

is satisfied.

Since we have $s = \frac{U_l + U_r}{2}$ which correspond to the shock wave speed, then for the point $(U_r, 0)$ we have $U = U_r$ and substitute in the previous inequality we get the left hand side of the inequality

$$(U_r - \frac{U_l + U_r}{2})^2 = (\frac{U_r - U_l}{2})^2$$

from the numerical simulation in Section 4 we have the following values

$$U_l = 0.75[m.s^{-1}], \quad U_r = 05[m.s^{-1}]$$

then the left hand side of the inequality equals to $0.39[m.s^{-1}]$.

Now we check the right hand side, we have $p(U) = 1 + U_r^2 = 1.25[m.s^{-1}]$ and $\delta = 1/\lambda$

where $\lambda = D * \beta = 0.1 \times 0.1$, then the right hand side equals to $0.05[m.s^{-1}]$, and $0.39 > 0.05$ then $U_r = 0.5[m.s^{-1}]$ satisfies the inequality condition and we claim that the point $(U_r, 0)$ is a stable node. Furthermore the point $(U_l, 1)$ is a saddle point. We can also claim that the point $(U_r, 0)$ acts as an attractor and we expect a heteroclinic orbit connecting the equilibrium points.

In the numerical simulation in Section 4, Figure 14 and Figure 17 shows the traveling wave solutions propagating with wave speed s equals to $0.625[m.s^{-1}]$.

4 Numerical Simulations

In this section, we discuss the Finite Volume method for the Burgers' equation (8) and discuss the Finite Difference method for the reaction diffusion equation (9). We have been shown that the numerical solution of the reaction diffusion equation (9) is stable under a small perturbation. We use MATLAB program to implement the numerical schemes.

4.1 Finite Volume method (FVM)

4.1.1 Background

FVM is popular numerical method for the approximate solution of partial differential equations(PDEs). If we compare FVM with finite difference method(FDM), the FVM has the following advantages [20]:

- Spatial discretisation is totally flexible:the mesh can accommodate to irregularly shaped boundaries to reduce geometric errors and the mesh can be refined locally to give more resolution in regions of particular interest.

- Equations are presented in integral form which are often as they are derived from the underlying physical laws.

- Because of the previous point there is no need for dependent variables to be differentiable everywhere which means that a larger class of problems can be solved.

- The FVM naturally conserves conserved variables when applied to PDEs expressing conservation laws since, two neighboring cells share a common interface, the total flow of a conserved quantity out of one cell will be the same as it is entering the other cell.

The main disadvantage of FVM that there is no solid theory that can explain the accuracy of the scheme produced by FVM. However a FVM in a uniform Cartesian mesh can be treated as a FDM which depend on Taylor series to estimate the accuracy condition. So we used heuristic formula to establish the accuracy of the scheme based on experimental results as we shall see later on in subsection 4.1.4
By writing the equation (9) as follow:

$$\partial_t u + \nabla.\underline{H} = 0 \tag{36}$$

Where $\nabla = i\frac{\partial}{\partial x} + j\frac{\partial}{\partial y}$ is the vector differential operator and $\underline{H} = Fi + Gj$ with $F = \frac{u^2}{2}$ and $G = 0$ while the equation (8) is one dimensional.
Then equation (36) is the starting point for the finite volume method which is written in conservative form.
Integrating (36) over an arbitrary region R gives:

$$\iint\limits_R (\frac{\partial u}{\partial t} + \nabla.H)dR = 0 \tag{37}$$

Then, we have

$$\iint\limits_R \frac{\partial u}{\partial t}dR + \iint\limits_R \nabla.HdR = 0 \tag{38}$$

Using one form of the Greens's theorem, the second integral in (38) can be replaced by a line integral around the boundary of the region R, we get

$$\iint\limits_R \frac{\partial u}{\partial t}dR + \oint\limits_C \underline{H}.\underline{n}ds = 0 \tag{39}$$

Where $\underline{n}$ is the outward pointing unit normal vector to R at any point on the curve C. We define $\overline{u}$ as the average value of u over the region R, then the integral of the time derivative term in equation (39) gives

$$A\frac{\partial \overline{u}}{\partial t} + \oint\limits_C \underline{H}.\underline{n}ds = 0 \tag{40}$$

Where A is the area of the region R and later on we shall consider it as Δx for the 1-D case. Rewriting (40) gives

$$\frac{\partial \overline{u}}{\partial t} = -\frac{1}{A} \oint\limits_{C} \underline{H}.\underline{n} ds \tag{41}$$

Equation (41) is a semi- integral form of (8) and applies to any region in the plane over which (9) holds.

Next, we define the mesh or the grid by dividing the domain into a finite number of polygonal cells. Since we deal with a 1-D case we have chosen the polygonal shape to be rectangular with a fixed size. This means that we use structured mesh cells. Structured mesh cells lead to a significant decrease in the computation time. We may also use unstructured mesh cells for more complex geometries.

The approximation of (41) over the mesh cells is done by a forward difference in time, then we get

$$\frac{u_i^{n+1} - u_i^n}{\Delta t} = -\frac{1}{A} \sum_{sides} \underline{H}^n.\underline{S} \tag{42}$$

where the integral term in (41) is approximated by the total sum of the fluxes over the cell interfaces, Δt is the time difference between two time levels indicated by n and i is the spatial grid size index. A is the cell area and S is the outward pointing normal vector whose length is the length of the cell side and is called a side vector. $\underline{H}^n$ is the flux through the cell interface which is constant along the cell side see Figure 7.

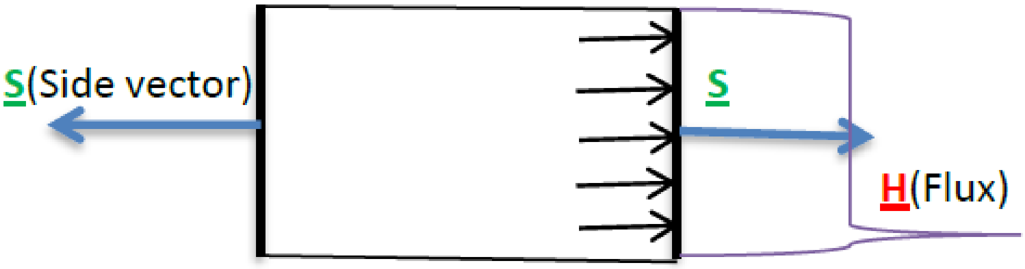

Figure 7: Side vectors over Computational cell

4.1.2 Finite Volume scheme (FVS) for Burgers' equation

We start from the equation (42) by defining the side vectors $\underline{S}$ and the fluxes through the interfaces as shown in Figure 7.

The side vectors in Cartesian mesh

$$S_{i+1/2} = \Delta y i + 0j \tag{43}$$

$$S_{i-1/2} = -\Delta y i + 0j \tag{44}$$

and

$$\underline{H} = Fi + Gj \tag{45}$$

where $F = \frac{u^2}{2}$ and $G = 0$

From equations (42)-(45) we get

$$u_i^{n+1} = u_i^n - \frac{\Delta t}{\Delta x}(F_{i+1/2}^n - F_{i-1/2}^n) \tag{46}$$

where $F_{i+1/2}^n$, $F_{i-1/2}^n$ are the fluxes in x direction at the cell interfaces.

From equation (46) we see that the fluxes at the interfaces can be approximated by the flux values at two neighboring cell centers .

$$F_{i+1/2} = \frac{F_{i+1} + F_i}{2} \tag{47}$$

$$F_{i-1/2} = \frac{F_i + F_{i-1}}{2} \tag{48}$$

From equations (46)-(48) we get:

$$u_i^{n+1} = u_i^n - \frac{\Delta t}{2\Delta x}(F_{i+1}^n - F_{i-1}^n) \tag{49}$$

Since $F = \frac{u^2}{2}$, then we can write (49) as follows:

$$u_i^{n+1} = u_i^n - \frac{\Delta t}{4\Delta x}(u_{i+1}^n - u_{i-1}^n) \tag{50}$$

The FVS (50) is identical to the classical forward in time backward in space(FTBS) but is unfortunately unconditionally unstable scheme. To stabilize it we use Lax-Friedrichs approach and write eq.(50) with central difference in time which gives

$$u_i^{n+1} = \frac{u_{i+1}^n + u_{i-1}^n}{2} - \frac{\Delta t}{4\Delta x}({u_{i+1}^n}^2 - {u_{i-1}^n}^2) \tag{51}$$

Equation (51) represents the FVS of the Burgers' equation (8) and implemented by MATLAB program.

4.1.3 Boundary condition

Lax- Friedrichs scheme (51) needs a ghost cell extended to the left and the right of the domain. We use a transmissive (zero gradient) boundary condition by inserting a ghost cell to the left and to the right of the domain and copies them from its neighbor cell(i.e.).. if we denote to the left ghost cell by $u(1)$ and the right gohst cell by $u(N)$ where N is the number of computational cells then we have

$$u(1) = u(2), \qquad\qquad u(N) = u(N-1)$$

4.1.4 Heuristic time step for FVS (51)

FVM, no theory guarantees the stability of the numerical scheme as for the FDM. By using a heuristic time step condition, our FVS (51) perform well under the following time step condition

$$\Delta t \leq \frac{\Delta x}{max|u|}$$

Our numerical stability condition is equivalent to the heuristic time step condition used for SWE in [20].

4.2 Finite Difference method(FDM)

4.2.1 Background

A Finite Difference method proceeds by replacing the derivatives in the differential equations with finite difference approximations. This gives a large finite algebraic system of equations to be solved instead of the partial differential equation, and it can be done by computer.

We should ask our self how we can approximate the derivatives of a known function by finite difference formula based only on values of the function itself at discrete points (grid points). And what we can say about the order of accuracy of an approximation in the simplest possible way.

For example, Let $f(x,t)$ is a function of two variables and always assumed to be smooth, meaning that we can differentiate the function several times and each derivative is a well defined.

Suppose that we want to approximate $\partial_x f(\overline{x},t)$ by finite difference approximation based only on the values of f at finite number of points near $\overline{x}$ one can choose the following option

$$\partial_x(f(\overline{x},t) \approx \frac{f(\overline{x}+h,t)-f(\overline{x},t)}{h} \tag{52}$$

$$\partial_x(f(\overline{x},t) \approx \frac{f(\overline{x},t)-f(\overline{x}-h,t)}{h} \tag{53}$$

for some value of h which is called a spatial difference between two grid points. Eq.(52) is called forward finite difference and eq.(53) is called backward finite difference.

For more options about the type of the finite approximation see Table (4.2.1).

The truncation error is so important in order to estimate the accuracy of the finite difference approximation. The standard approach for analyzing the error in a finite difference approximation is to expand each of the function values of f in *Taylor* *expansions* around the point $\overline{x}$

$$f(\overline{x}+h) = f(\overline{x}) + hf'(\overline{x}) + \frac{h^2}{2!}f''(\overline{x}) + \frac{h^3}{3!}f'''(\overline{x}) + O(h^4) \tag{54}$$

This expression is valid since f is assumed to be sufficiently smooth. For more about estimating the error or the order of accuracy of the finite difference approximations method we refer to [21].

partial derivative	finite difference approximation	type	order
$\frac{\partial c}{\partial x} = c_x$	$\frac{c_{i+1}^n - c_i^n}{\Delta x}$	forward	first in x
$\frac{\partial c}{\partial x} = c_x$	$\frac{c_i^n - c_{i-1}^n}{\Delta x}$	backward	first in x
$\frac{\partial c}{\partial x} = c_x$	$\frac{c_{i+1}^n - c_{i-1}^n}{2\Delta x}$	central	second in x
$\frac{\partial^2 c}{\partial x^2} = c_{xx}$	$\frac{c_{i+1}^n - 2c_i^n + c_{i-1}^n}{\Delta x^2}$	symmetric	second in x
$\frac{\partial c}{\partial t} = c_t$	$\frac{c_i^{n+1} - c_i^n}{\Delta t}$	forward	first in t
$\frac{\partial c}{\partial t} = c_t$	$\frac{c_i^n - c_i^{n-1}}{\Delta t}$	backward	first in t
$\frac{\partial c}{\partial t} = c_t$	$\frac{c_i^{n+1} - c_i^{n-1}}{2\Delta t}$	central	second in t
$\frac{\partial^2 c}{\partial t^2} = c_{tt}$	$\frac{c_i^{n+1} - 2c_i^n + c_i^{n-1}}{\Delta t^2}$	central	second in t

Table 3: Toolkit

4.2.2 Finite Difference Scheme(FDS) for Eq.(9)

By using the information in Table (4.2.1) with some support from [22] [23], we can write down the reaction diffusion equation (9) in its discrete form as follows:

$$\begin{aligned} c_i^{n+1} &= c_i^n + \frac{\lambda \Delta t}{\Delta x^2}(P^n_{i+\frac{1}{2}}(c^n_{i+1} - c^n_i) - P^n_{i-\frac{1}{2}}(c^n_i - c^n_{i-1})) \\ &+ (\frac{\Delta t}{\Delta x})u^n_i(c^n_{i+1} - c^n_i) + \Delta t c^n_i(1 - c^n_i). \end{aligned} \tag{55}$$

with

$$\begin{aligned} P^n_{i+\frac{1}{2}} &= P(x + \frac{1}{2}, t_n) = 1 + u(x + \frac{1}{2}, t_n)^2 = P(\frac{x_{i+1} + x_i}{2}, t_n), \\ P^n_{i-\frac{1}{2}} &= P(x - \frac{1}{2}, t_n) = 1 + u(x - \frac{1}{2}, t_n)^2 = P(\frac{x_i + x_{i-1}}{2}, t_n) \end{aligned}$$

Where c^n_i denotes the approximation value of the chemical concentration $c(x,t)$ at a spatial grid point i and time level n. We require u to be approximated at the cell center and this is provided by the finite volume scheme (51). The time step size is Δt and Δx is the spatial grid size.

Equation (55) represents an explicit finite difference scheme (FDS) for the reaction diffusion equation (9) and it can be seen from Figure 8.

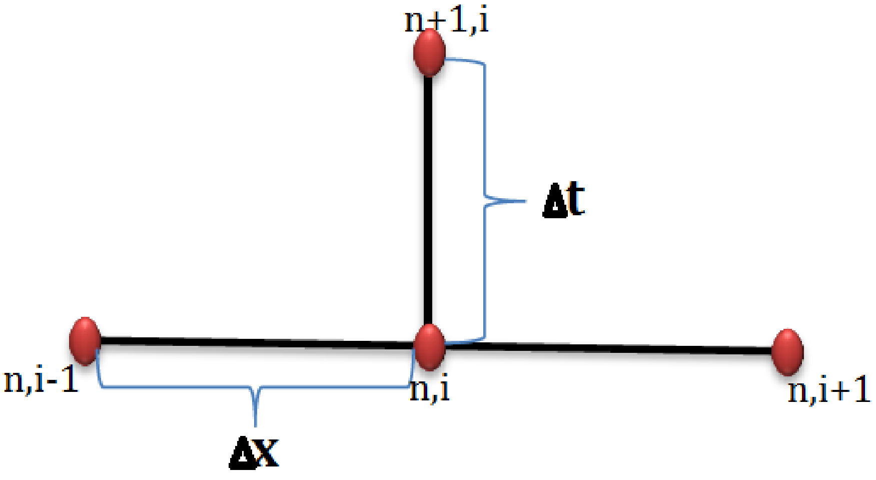

Figure 8: Grid point stencil

4.2.3 Stability condition for FDS (55)

In this part we discuss the stability condition for the finite difference scheme (55) in the spirit of the lectures given by *J. Struckmeier*, summer term 2011, University of Hamburg [23]. The FDS (55) leads to the following

$$\begin{aligned} e_i^{n+1} &= e_i^n + \frac{\lambda \Delta t}{\Delta x^2}(P_{i+\frac{1}{2}}^n(e_{i+1}^n - e_i^n) - P_{i-\frac{1}{2}}^n(e_i^n - e_{i-1}^n)) \\ &+ (\frac{\Delta t}{\Delta x})u_i^n(e_{i+1}^n - e_i^n) - \Delta t T_i^n \end{aligned} \tag{56}$$

where e is the error and T is the truncation error with $\nu = \frac{\Delta t}{\Delta x^2}$ and $\mu = \frac{\Delta t}{\Delta x}$. By arrangement the previous equation we get

$$\begin{aligned} e_i^{n+1} &= e_i^n + \lambda\nu(P_{i+\frac{1}{2}}^n e_{i+1}^n - (P_{i+\frac{1}{2}}^n + P_{i-\frac{1}{2}}^n)e_i^n - P_{i-\frac{1}{2}}^n e_{i-1}^n) \\ &+ \mu u_i^n(e_{i+1}^n - e_i^n) - \Delta t T_i^n \\ &= (1 - \nu\lambda(P_{i+\frac{1}{2}}^n + P_{i-\frac{1}{2}}^n) - \mu u_i^n)e_i^n \\ &+ (\nu\lambda P_{i+\frac{1}{2}}^n + \mu u_i^n)e_{i+1}^n \\ &+ (\nu\lambda P_{i-\frac{1}{2}}^n)e_{i-1}^n - \Delta t T_i^n \end{aligned} \tag{57}$$

In order to estimate the stability condition of the FDS (55) we need to ensure that all the coefficients on the right hand side of the equation (57) are non-negative, which means

$$\nu\lambda(P_{i+\frac{1}{2}}^n + P_{i-\frac{1}{2}}^n) + \mu u_i^n \leq 1 \tag{58}$$

From equation (58) we have no restriction on the spatial step size Δx but rather this requires a more severe restriction on the size of the time step. Unfortunately the forward difference approximation of the advection term introduces an error of order Δx instead of the order $(\Delta x)^2$ given by the central difference. This can be consider as the price we have to pay in order to eliminate the restriction on the spatial step size.

Now we can write the stability condition of the FDS (55) as follows

$$\Delta t \leq \frac{\Delta x^2}{\lambda(P^n_{i+\frac{1}{2}} + P^n_{i-\frac{1}{2}}) + \Delta x u^n_i}$$

4.3 Numerical simulations results

In this subsection, we show some numerical simulations for the model (8),(9) to verify our theoretical results. In this simulation we set the following initial conditions:

$$\begin{aligned} c(x,0) &= c_0(x) = 0.05^*\gamma/(1+exp(2^*(x-\eta))), \qquad 0 < x < L \\ u(x,0) &= U_l = 0.75[m.s^{-1}] \quad 0 \leq x \leq 20 \;\; \& \\ u(x,0) &= U_r = 0.5[m.s^{-1}] \quad 20 < x \leq L \end{aligned} \tag{59}$$

with boundary conditions for the reaction diffusion equation, the left and right states of the concentration c are given by 1 and 0, respectively. That is for $t = 0.3[s]$

$$\begin{aligned} c_l &= 1 \qquad 0 \leq x \leq 40 \;\; \& \\ c_r &= 0 \qquad x \geq 40 \end{aligned} \tag{60}$$

The plot of the initials data of the model (8),(9) are given in Figure 9 and Figure 10.

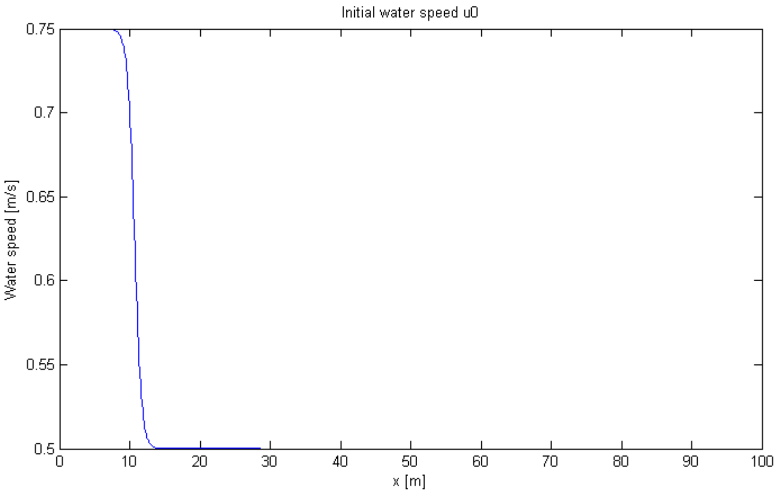

Figure 9: Initial water speed

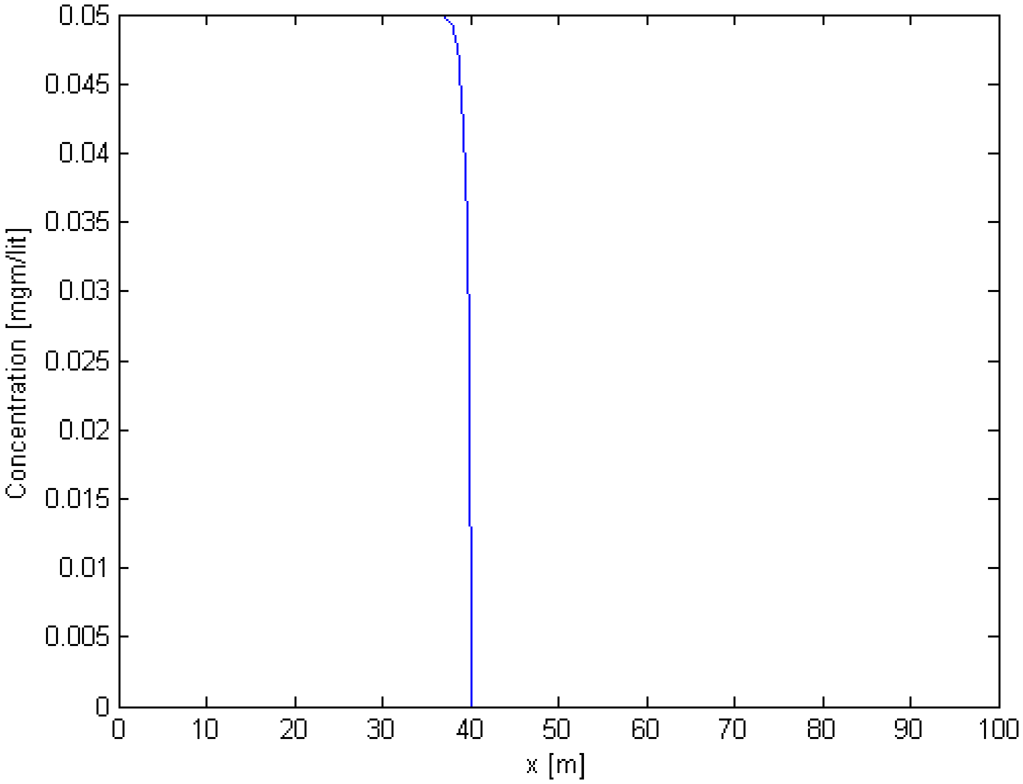

Figure 10: Plot of initial concentration function with $\eta = 40, \gamma = 1$

Figure (11) shows a shock wave profile for Burgers' equation (8) which evolves with time t, this result is totally agrees with the theoretical point of view in Section (2).

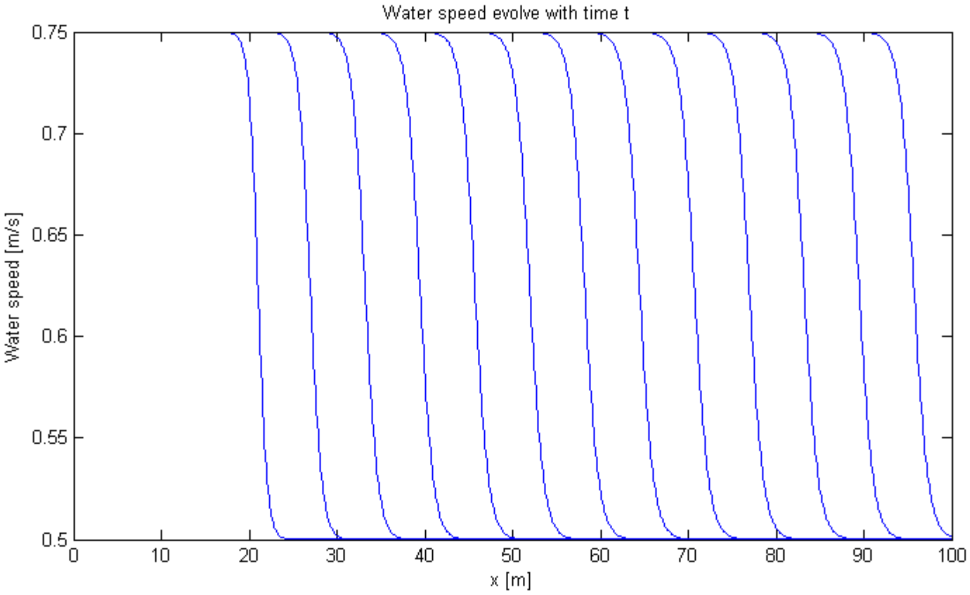

Figure 11: Shock profile for the water speed evolves with time

For the reaction diffusion equation when the time is less than 0.3 second we get the results shown in Figure (12) which correspond to the fact that the chemical reaction rate of the sulfuric acid with the water is $0.3 sec^{-1}$.

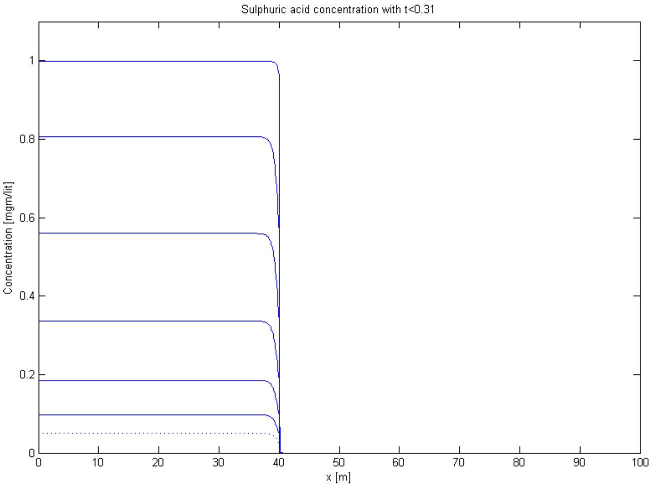

Figure 12: Chemical concentration with time $t \leq 0.3$ and $\eta = 40, \gamma = 20$

For the case when $t > 0.3$ we can see from Figure 13 a heteroclinic acts as a front wave profile, which propagates with wave speed $s = 0.625[m.s^{-1}]$ and evolves with the time and this agrees with the analysis performed in Section (2).

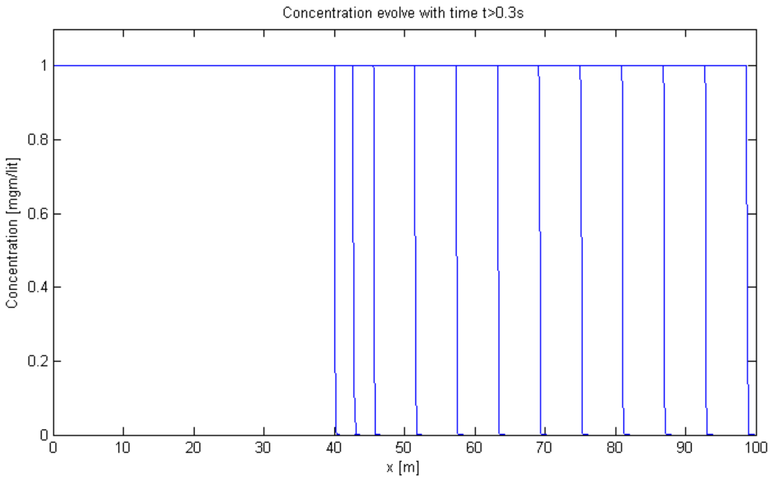

Figure 13: Chemical concentration evolves with time $t > 0:3$ and $\eta = 40$, $\gamma = 20$.

Figure (14) shows that the concentration profile evolves with time $t > 0$

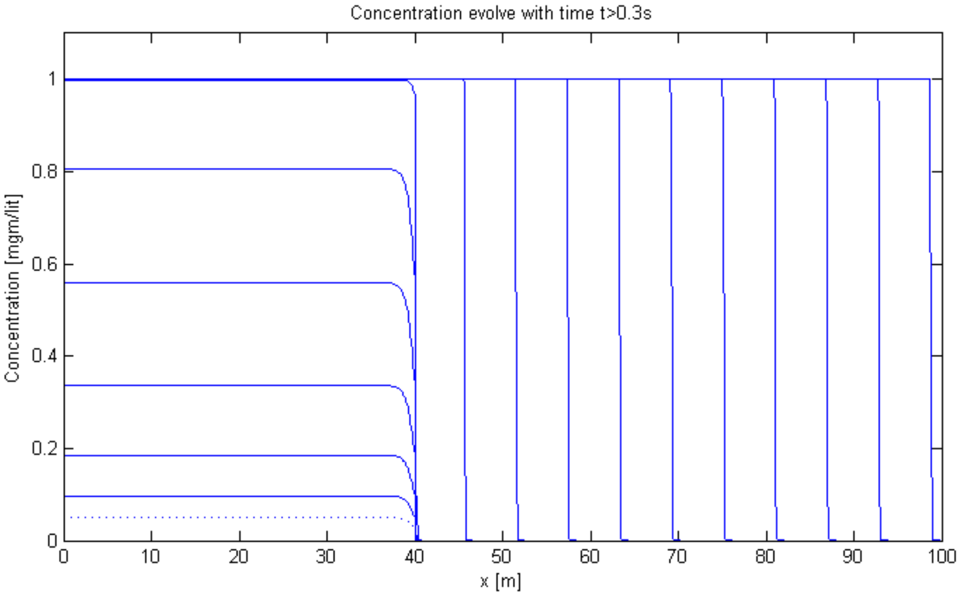

Figure 14: Concentration evolve with time $t > 0$

4.4 Stability of the numerical solution

In this part, we focus on the solution of the reaction diffusion equation (9). We apply a small perturbation to the initial concentration in order to examine either the solution of the reaction diffusion equation (9) is stable under this small perturbation or it blows up and shows instability.
The initial perturbation is given by

$$\bar{c}_0 = \frac{0.5 \sin x}{(\frac{x-80}{10})^2 + 1} \tag{61}$$

Figure (15) represents the plot of the initial concentration under a small perturbation

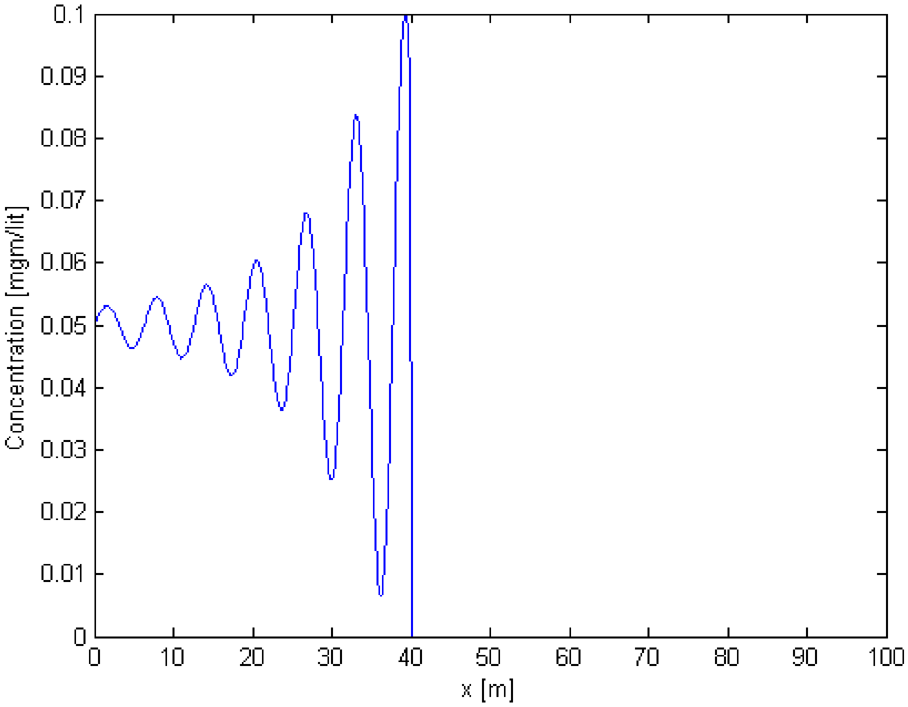

Figure 15: Initial concentration with small perturbation

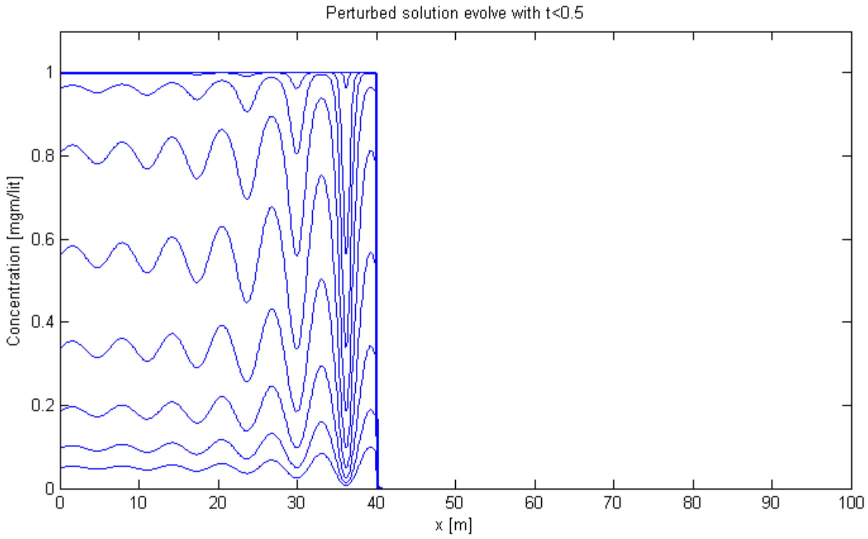

Figure 16: Concentration evolves under a small perturbation with $t < 0.3$

Figure (16) shows the evolution of the perturbed solution of a reaction diffusion equation with $t \leq 0.5$ and Figure 17 shows that the perturbation disappears completely after reaching the equilibrium point 1 in time less than $0.3[s]$.

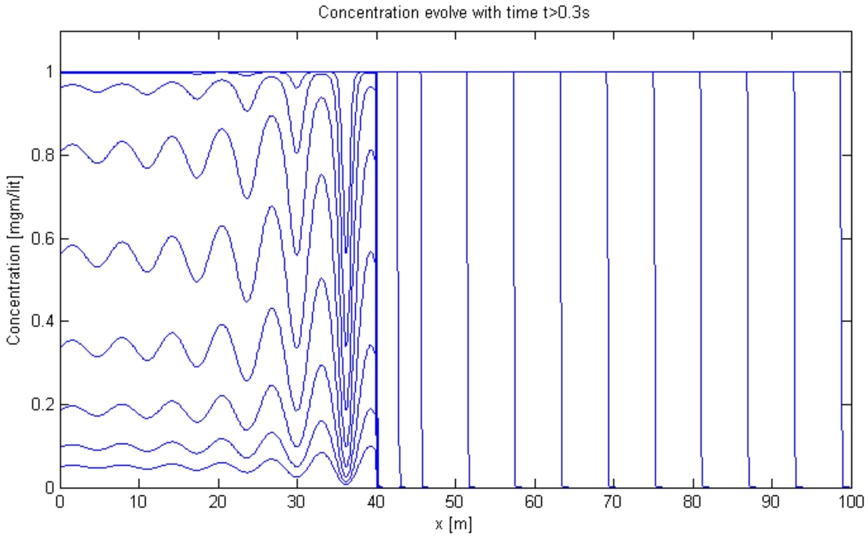

Figure 17: Concentration c evolves with time t

5 Conclusion and future scope

We established the verification of a traveling wave solutions of the reaction diffusion equation coupled with shallow water equations. The advection and diffusion coefficients are dependent on the water flow velocity u and consequently we have a coefficients which it changes with time t and space x. For simplicity, we reduce the shallow water equation into Burgers' equation which gives the water velocity profile in the river and from the numerical simulation we have seen the shock wave profiles which acts as a traveling wave solution of the Burgers' equation.

By using the phase plane analysis we conclude that there exists a traveling wave solutions of our model if the inequality $(U - s)^2 \geq \pm 4p(U)/\delta$ hold for all possible values of U as shown in Section (3).

We observe from the numerical simulation that how good is the analytical analysis to show the existence of traveling wave solutions of the system (4)-(5), where we can easily see from the numerical part that for the Burgers' equation we have a shock profile in a nice form. Furthermore, we observe the traveling wave solution of the reaction diffusion equation, which moves with speed $s = 0.625[m.s^{-1}]$.

To investigate the stability of the numerical solution for the reaction diffusion equation solution, we apply small perturbation in the initial data. We observe that the numerical solution of the reaction diffusion equation is stable under this small perturbation, where the perturbation disappeared within $0.3[s]$ and the solution is almost as the normal solution without perturbation.

In this thesis we did not address the stability of the traveling wave solutions of the reaction diffusion equations analytically and it is left for future work. In the future, we may consider more general model of the incident we studied while we can consider the impact of the air pollutants and the affects of these kind of pollutants into the environment inside the rivers.

For more accuracy in the numerical simulation we may use a modern technology to observe the natural hazards and estimate the measurements rather than only relying on the classical ways. For example, in our incident no real measurements are available because of difficulty to measure the concentration of sulfuric acid in its violent reaction. But if we can measure it remotely it could be a great chance to enhance our numerical simulation, and this can be obtain by using satellite images.

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