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Travelling wave solutions of a Reaction-Diffusion System: Slow Reaction and Slow Diffusion

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Abstract: - In this paper we study the travelling wave solutions of a reaction-diffusion system with a slow reaction and a slow diffusion for one component. We use a semi-implicit method and finite element method (COMSOL software) for solving this system. We compare both methods and we found an excellent agreement between the solutions.

Keywords: - *Reaction-Diffusion, Travelling wave solutions, Numerical methods*

I. INTRODUCTION

Traveling wave is a wave that move with constant speed without changes of its shape (see for example [9,10]). A Reaction-Diffusion models have many applications in biology, chemistry, ecology and physics. The travelling wave solutions are the key fact to translate these applications to a mathematical equations see [4-8]. One of the reaction-diffusion model has been derived from the reaction between two chemical species A and B that react via the single autocatalytic step

$A + B \to 2B,$ rate kab, where $a = [A]$ and $b = [B]$. The mathematical system that derived from these interactions is the governing equations for the one-dimensional chemical system [1,2],

$$\frac{\partial u}{\partial t} = D_u\, \lambda \frac{\partial^2 u}{\partial x^2} - k_u \lambda\, uw,$$
$$\frac{\partial w}{\partial t} = D_w\, \frac{\partial^2 w}{\partial x^2} + k_w uw, \quad \dots\dots (1)$$

where $-k_u\ \lambda uw, k_w uw,$ are the reaction terms and the rests of the terms are the diffusion terms, amd $\lambda \ll 1$, k_u , k_w are positive. The travelling wave connects stable steady states to other states. When $\lambda \ll 1$, the equation of u has a slow reaction and slow diffusion. It was shown in [1] that when $\lambda = 1$ there exists a travelling wave solution in (1) that connects a stable steady state (1,0) to (0,1) . In the section 2, we use a finite difference method to solve (1) and find the traveling wave solutions, in section 3, we use COMSOL finite element method package to solve the reaction diffusion system and compare it to the numerical method in section 2. We conclude in section 4. We assume in what follows $k_u = k_w = 1$.

II. NUMERICAL METHODS

In this section we solve (1) numerically and try to find the travelling wave solutions that connect (1,0) to (0,1) and generated by the initial conditions. A semi-implicit finite difference method provides a sufficiently accurate numerical solution since it is unconditionally stable. An implicit method is used to discretise the diffusion operator. For the non linear reaction part we use an explicit method. Finite difference method can be derived using Taylor series expansion $u(x_0 + \Delta x)$ and $u(x_0 - \Delta x)$, where Δx is the step size of x. The discretization equation of (1) is

$$\frac{u_n^{t+\Delta t} - u_n^t}{\Delta t} = \lambda \frac{u_{n+\Delta x}^{t+\Delta t} - 2u_n^{t+\Delta t} + u_{n-\Delta x}^{t+\Delta t}}{(\Delta x)^2} - \lambda u_n^t (u_n^t w_n^t)\ ,$$
$$\frac{w_n^{t+\Delta t} - w_n^t}{\Delta t} = D\, \frac{w_{n+\Delta x}^{t+\Delta t} - 2w_n^{t+\Delta t} + w_{n-\Delta x}^{t+\Delta t}}{(\Delta x)^2} + w_n^t (u_n^t w_n^t)\ ,$$

These equations simplify to give us

$$D\lambda r u_{n+\Delta x}^{t+\Delta t} - (1 + 2\lambda r) u_n^{t+\Delta t} + rD\lambda u_{n-\Delta x}^{t+\Delta t} = -u_n^t + (\Delta t)\lambda u_n^t (u_n^t w_n^t)\ ,$$
$$r\, w_{n+\Delta x}^{t+\Delta t} - (1 + 2Dr) w_n^{t+\Delta t} + r w_{n-\Delta x}^{t+\Delta t} = -w_n^t - (\Delta t) w_n^t (u_n^t w_n^t)\ ,$$

where $r = \frac{\Delta t}{(\Delta x)^2}$. The domain of solution $0 < x < l$ is divided into N discrete equally spaced points $x = x_i = (i - 1)\Delta x$, where $i = 1,2, \dots, N$ and $\Delta x = l/(N - 1)$. The length of domain l should be much larger than $O\left(\frac{1}{\lambda}\right)$, when $\lambda \ll 1$ to capture the travelling wave solutions. The initial conditions are $u(x, 0) = u_0(x)$ and $w(x, 0) =$

$w_0(x)$. The boundary conditions are no flux Neumann boundary, $u_x = w_x = 0$ at $x = 0, l$, which are imposed using three point formula (this is a second order accuracy stable).

$u'(x) = \frac{-3u_n^{t+\Delta t} + 4u_{n+\Delta x}^{t+\Delta t} - u_{n+2\Delta x}^{t+\Delta t}}{2\Delta x} = 0$,

$w'(x) = \frac{-3w_n^{t+\Delta t} + 4w_{n+\Delta x}^{t+\Delta t} - w_{n+2\Delta x}^{t+\Delta t}}{2\Delta x} = 0.$ 2.1

From discretization we get a system of algebraic equations which can be written in the form

$AU^{t+1} = bU^t$ 2.2

$BW^{t+1} = cW^t$

$$\begin{bmatrix} 3 & -4 & 1 & \\ -r & (1+2D\lambda r) & -r & \\ \ddots & \ddots & \ddots & \\ & -r & (1+2D\lambda r) & -r \\ & 1 & -4 & 3 \end{bmatrix} \begin{bmatrix} u_1^{t+1} \\ u_2^{t+1} \\ \vdots \\ u_{N-1}^{t+1} \\ u_N^{t+1} \end{bmatrix} = \begin{bmatrix} 0 \\ u_2^t + (\Delta t)\lambda u_2^t (u_2^t (w_2^t)^k) \\ \vdots \\ u_{N-1}^t + (\Delta t) u_{N-1}^t \lambda (u_{N-1}^t (w_{N-1}^t)^k) \\ 0 \end{bmatrix},$$

Where

$$A = \begin{pmatrix} 3 & -4 & 1 & \\ -D\lambda r & (1+2D\lambda r) & -D\lambda r & \\ \ddots & \ddots & \ddots & \\ & -D\lambda r & (1+2D\lambda r) & -D\lambda r \\ & 1 & -4 & 3 \end{pmatrix}$$

$$bU^t = \begin{bmatrix} 0 \\ u_2^t - (\Delta t) u_2^t (u_2^t (w_2^t)^k) \\ \vdots \\ u_{N-1}^t - (\Delta t) u_{N-1}^t (u_{N-1}^t (w_{N-1}^t)^k) \\ 0 \end{bmatrix}, \quad U^{t+1} = \begin{bmatrix} u_1^{t+1} \\ u_2^{t+1} \\ \vdots \\ u_{N-1}^{t+1} \\ u_N^{t+1} \end{bmatrix}$$

In the case of w

$$B = \begin{pmatrix} 3 & -4 & 1 & \\ -r & (1+2r) & -r & \\ \ddots & \ddots & \ddots & \\ & -r & (1+2r) & -r \\ & 1 & -4 & 3 \end{pmatrix}$$

$$cW^t = \begin{bmatrix} 0 \\ w_2^t + (\Delta t) w_2^t (u_2^t w_2^t) \\ \vdots \\ w_{N-1}^t + (\Delta t) w_{N-1}^t (u_{N-1}^t w_{N-1}^t) \\ 0 \end{bmatrix}, \quad W^{t+1} = \begin{bmatrix} w_1^{t+1} \\ w_2^{t+1} \\ \vdots \\ w_{N-1}^{t+1} \\ w_N^{t+1} \end{bmatrix}$$

The initial condition that is used for solving (2.1) and (2.2) are,

$$u(x,0) = 1 + \tanh(x),$$
$$w(x,0) = 1 - \tanh(x),$$

We solve the linear system (2.2) and (2.3) at each time step using the backslash operator in MATLAB.

III. RESULTS AND DISCUSSION:

We applied our codes to the problem (1) when $\boldsymbol{\lambda} = \mathbf{1}, \boldsymbol{D} = \mathbf{1}$, and we get the same results as in [1]. For $\boldsymbol{\lambda} \ll \mathbf{1}$, the results shown in Fig. (1), explains the travelling wave solutions for both $\boldsymbol{u}$ and $\boldsymbol{w}$ when $\boldsymbol{D} = \mathbf{1}$. It is clear that with small $\boldsymbol{\lambda} \ll \mathbf{1}$, the traveling wave of $\boldsymbol{w}$ grows exponentially and there is no effects on $\boldsymbol{u}$. The travelling wave solutions are also found for this system using COMSOL, the finite element tool (for more details about COMSOL see [3]) as shown in Fig. (2-3). A comparison between these results in the two methods has shown first in Fig. (4) for $\boldsymbol{u}$, and for $\boldsymbol{w}$ in Fig. (5). Finally, a comparison between the travelling wave solution in the two methods for $\boldsymbol{u}$ and $\boldsymbol{w}$ is shown in Fig. (6). From these figures its clear that there are an excellent agreement between the results in both methods.

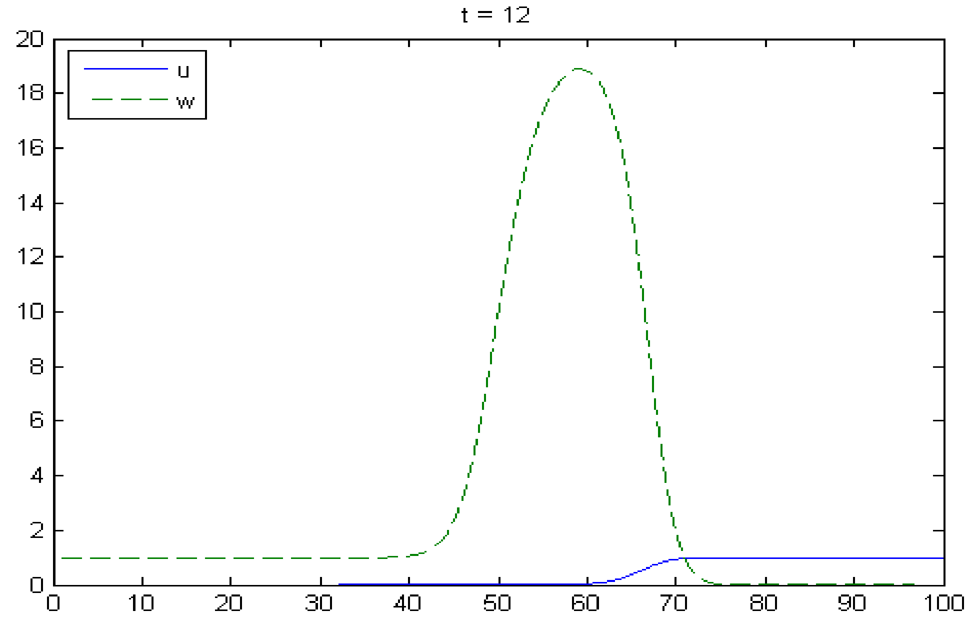

Figure 1: Travelling wave solutions for $\boldsymbol{u}$ and $\boldsymbol{w}$ in (1) from semi-implicit method.

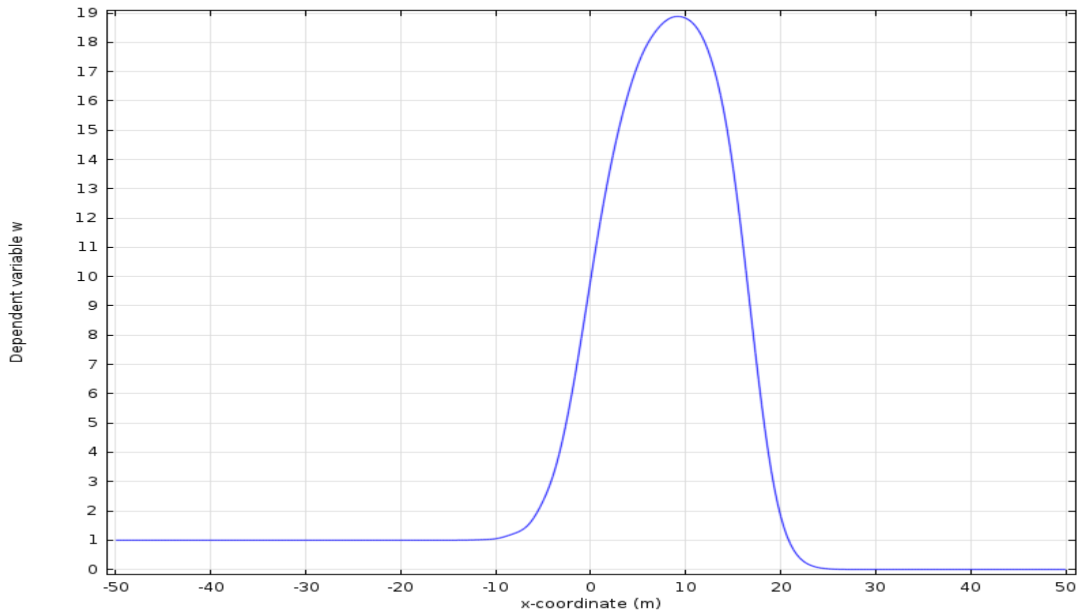

Figure 2: Travelling wave solutions for $\boldsymbol{u}$ in (1) from COMSOL finite element solution.

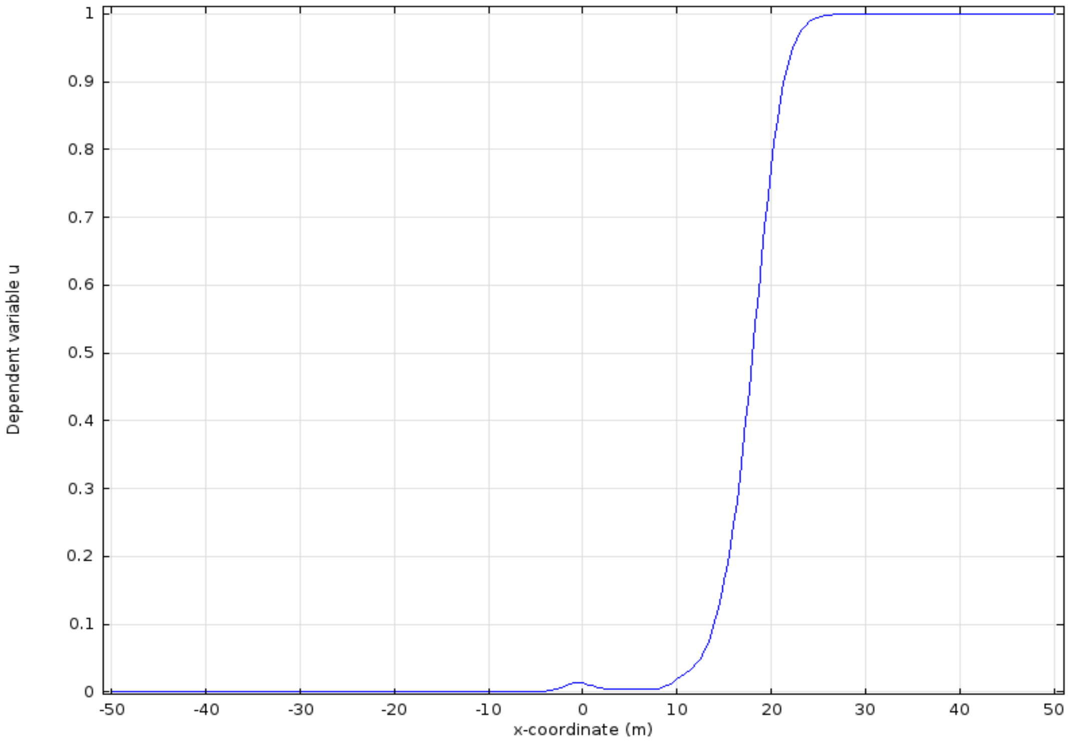

Figure 3: Travelling wave solutions for $\boldsymbol{w}$ in (1) from COMSOL finite element solution.

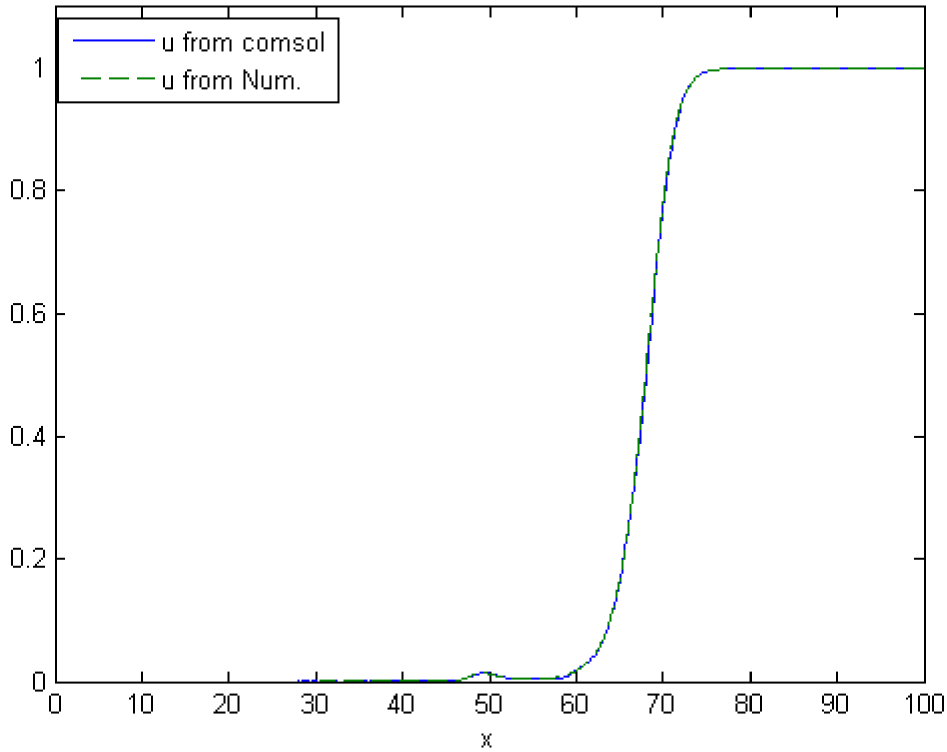

Figure 4: Comparison between travelling wave solutions for $\boldsymbol{u}$ in (1) in both methods.

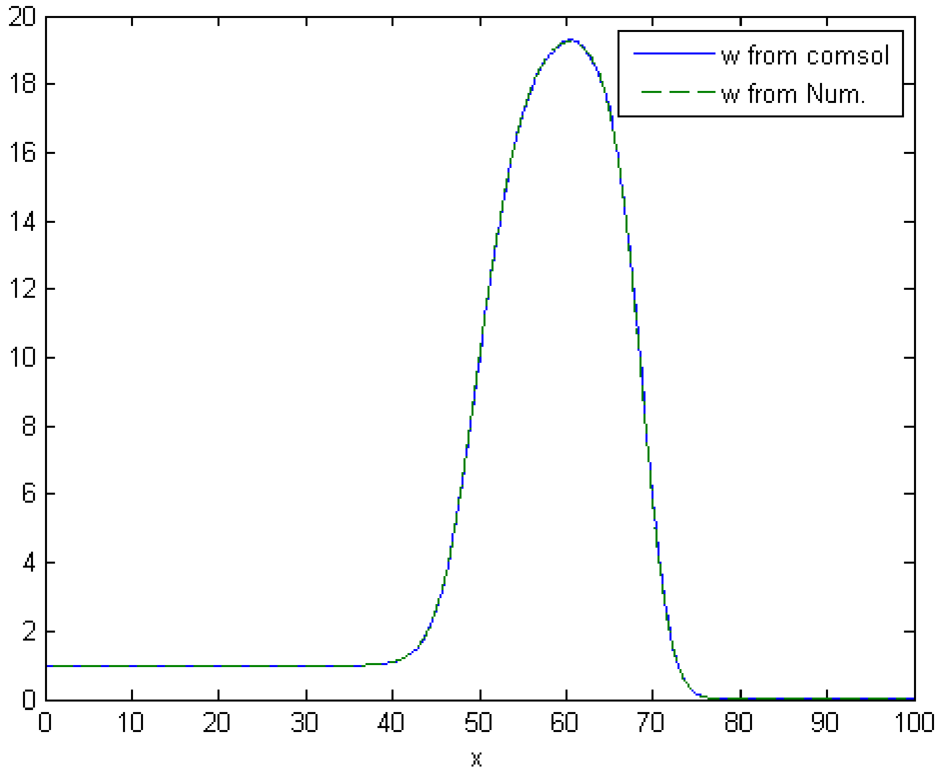

Figure 5: Comparison between travelling wave solutions for $\boldsymbol{w}$ in (1) in both methods.

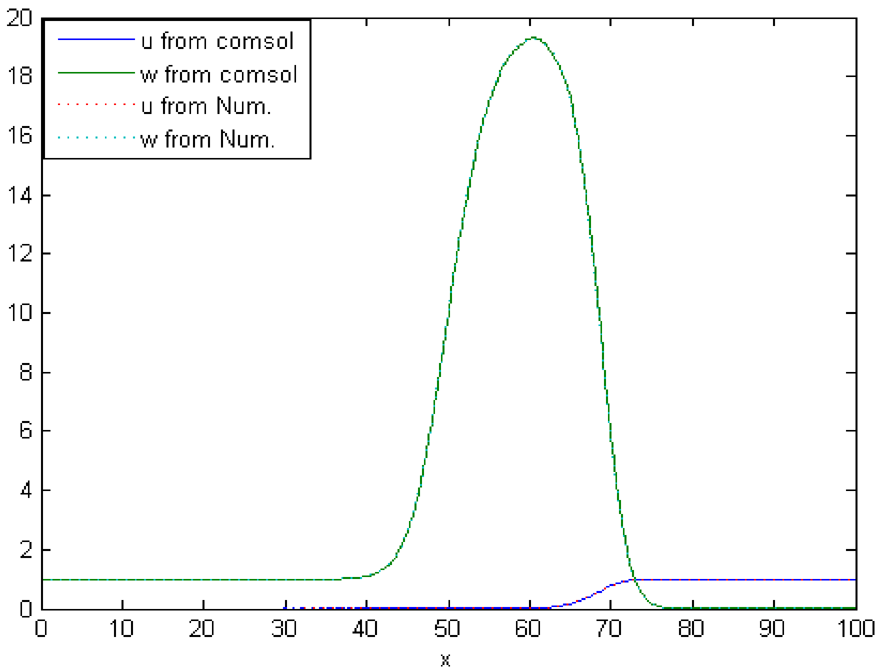

Figure 6: Comparison between travelling wave solutions for $\boldsymbol{u}$ and $\boldsymbol{u}$ in (1) in both methods.

IV. CONCLUSIONS

We have found the travelling wave solution for the reaction-diffusion system (1) using semi-implicit method and finite element method. It has been found that for slow reaction and diffusion, the traveling wave of $\boldsymbol{w}$ grows exponentially and there are no effects on the wave $\boldsymbol{u}$. The results are agree in both methods.

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