A Crank-Nicolson Method of Autocatalytic Reaction-Diffusion Systems
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ABSTRACT
In this paper we used two numerical methods to investigate propagating heat solutions of PDEs. The explicit and Crank-Nicolson methods and the results show that Crank-Nicolson method is more accurate than the explicit method. As an illustration, we used the above method to an autocatalytic reaction diffusion equations involving two diffusing chemicals in one dimension.

Keywords: Crank-Nicolson Method, explicit, autocatalytic reaction diffusion equations.

1. Introduction
Many systems in biology and chemistry are intrinsically oscillatory [10]. Chemical reactions are modeled by non-linear partial differential equations (PDEs) exhibiting travelling wave solutions [5]. These oscillations occur due to feedback in the system either chemical feedback (such as autocatalysis) or temperature feedback due to a non-isothermal reaction [1,7].

Two well-studied examples of reactions exhibiting oscillatory solutions are the isothermal Belousov-Zhabotinsky reaction and the Sal’nikov thermokinetic oscillator.

The Gray-Scott scheme, which presents cubic-autocatalysis with linear catalyst decay, has been much considered, because of its multiple...
steady-state response and oscillatory solutions. For review and descriptions of much of this work. The scheme is

\[ u + 2v \to 3v, \text{ rate } = \beta uv^2, \quad v \to w, \text{ rate } = \beta y, \quad (1.1) \]

Where the concentrations of the reactant and autocatalyst are u and v, respectively. The parameters \( \beta \) and \( \gamma \) are rate constants. The catalyst is not stable, but undergoes a simple linear decay to a product w. This allows a much wider variety of behavior in the system than does the cubic reaction alone [3,4]. The nonlinear phenomena may be due to feedback through the detailed chemical mechanism or through departure from the isothermal state [9]. A typical phenomena in above scheme consists of the oscillation of the concentrations of the reactant and the autocatalyst in the two regions. We now consider the following model. In region I, the reaction is given by a cubic autocatalyst together with a linear decay of the autocatalyst, to an intermediate product W. In region II, the reaction is given by a pure intergauge of the reactant through the two regions while the autocatalyst concentration is taken to be zero [1,8].

2. The Mathematical Model

The cubic-autocatalytic reaction with linear decay (1.1) is considered in a non-dimensional reaction-diffusion cell. The partial differential equations are:

\[
\begin{align*}
    u_t &= u_{xx} - \beta uv^2, \\
    v_t &= v_{xx} + \beta uv^2 - \beta y v \\
    u_x &= v_x = 0 \quad \text{at} \quad x = 0, \\
    u &= 1 \quad \text{at} \quad x = 1 \quad \text{and} \quad t = 0, \\
    v &= v_0
\end{align*}
\]

The system (2.1) is in non-dimensional form with the concentrations of the reactant and autocatalyst given by u and v, respectively. It is an open system; the reactor has a permeable boundary at \( x = 1 \). Joined to a reservoir which contains u and v at constant concentrations. The boundary condition at \( x = 0 \) is a symmetry condition, an identical reservoir is located at \( x = -1 \). The system is characterized by three non-dimensional parameters. The ratio of the autocatalyst and reactant concentrations in the reservoir is \( v_0 \). The parameter \( \beta \) is a measure of the importance of the reaction terms, compared with diffusion, while \( \gamma \) is a measure of the importance of autocatalyst decay, compared with the cubic-reaction. The simplest way to adjust the non-dimensional parameters experimentally is by changing the reservoir concentrations.
Other possibilities for varying the non-dimensional parameters include changing the diffusivity of the system or the length of the reactor. The diffusivity could be changed by adjusting the temperature or by the addition of otherwise inactive salts [6,7].

3. Numerical Method:

In this paper, we depended on the Crank-Nicolson and Explicit algorithms to solve the mathematical model in (2.1).

3.1 The Explicit Method:

Explicit method is another method to solve the system (2.1). Thus we get from (2.1a) [11].

\[
\frac{u_{i,j+1} - u_{i,j}}{\delta t} = \frac{u_{i+1,j} - 2u_{i,j} + u_{i-1,j}}{2\delta x^2} - \beta u_{i,j}(v_{i,j})^2
\]

also from (2.1b) we get

\[
\frac{v_{i,j+1} - v_{i,j}}{\delta t} = \frac{v_{i+1,j} - 2v_{i,j} + v_{i-1,j}}{2\delta x^2} + \beta u_{i,j}(v_{i,j})^2 - \beta \gamma v_{i,j}
\]

and 2.1c becomes

\[
\frac{u_{i+1,j} - u_{i-1,j}}{2\delta x} = 0 , \text{ at } x = 0
\]

and 2.1d is

\[
u_{i,j} = 1 \\
\text{at } x = 1 \text{ and } t = 0
\]

\[
v_{i,j} = v_0
\]

thus in general the system (2.1) becomes

\[
\begin{align*}
\text{u}_{1,j+1} &= (1 - 2r)u_{1,j} + 2ru_{2,j} - \beta \delta t (u_{1,j})(v_{1,j})^2 \\
\text{at } x = 0, i &= 1
\end{align*}
\]

\[
\begin{align*}
\text{u}_{i,j+1} &= ru_{i-1,j} + (1 - 2r)u_{i,j} + ru_{i+1,j} - \delta t \beta (u_{i,j})(v_{i,j})^2 \\
\text{at } 0 < x < 1, i &= 2,3,\ldots,10
\end{align*}
\]
\[ u_{i,j+1} = 1 \quad \text{at } x = 1, \ i = 11 \]
\[ v_{1,j+1} = (1 - 2r)v_{1,j} + 2rv_{2,j} + \beta \delta t (u_{1,j})(v_{1,j})^2 - \beta \delta t \gamma v_{1,j} \quad \text{at } x = 0, \ i = 1 \]
\[ v_{i,j+1} = rv_{i-1,j} + (1 - 2r)v_{i,j} + \delta t \beta (u_{i,j})(v_{i,j})^2 - \delta t \beta \gamma v_{i,j} \quad \text{at } 0 < x < 1, \ i = 2, 3, \ldots, 10 \]
\[ v_{i,j+1} = v_0 \quad \text{at } x = 1 \text{ and } i = 11 \]

\[ \left\{ \begin{array}{c}
2 \frac{u_{i,j+1} - u_{i,j}}{\delta t} = \frac{u_{i+1,j+1} - 2u_{i,j+1} + u_{i-1,j+1}}{2\delta x^2} + \frac{u_{i+1,j} - 2u_{i,j} + u_{i-1,j}}{2\delta x^2} - \beta u_{i,j}(v_{i,j})^2
\end{array} \right. \]

also from (2.1b) we get
\[ \frac{v_{i,j+1} - v_{i,j}}{\delta t} = \frac{v_{i+1,j+1} - 2v_{i,j+1} + v_{i-1,j+1}}{2\delta x^2} + \frac{v_{i+1,j} - 2v_{i,j} + v_{i-1,j}}{2\delta x^2} + \beta u_{i,j}(v_{i,j})^2 - \beta \gamma v_{i,j} \]

and 2.1c becomes
\[ \frac{u_{i+1,j} - u_{i-1,j}}{2\delta x} = \frac{v_{i+1,j} - v_{i-1,j}}{2\delta x} = 0, \text{ at } x = 0 \]

and 2.1d is
\[ u_{i,j} = 1 \quad \text{at } x = 1 \text{ and } t = 0 \]
\[ v_{i,j} = v_0 \]

Thus in general the system (2.1) becomes:
\[ \left\{ \begin{array}{c}
(2 + 2r)u_{1,j+1} - 2ru_{2,j+1} = (2 - 2r)u_{1,j} + 2ru_{2,j} - 2\beta \delta t (u_{1,j})(v_{1,j})^2 \quad \text{at } x = 0, \ i = 1
\end{array} \right. \]
A Crank-Nicolson Method

-ru_{i-1,j+1} + (2 + 2r)u_{i,j+1} - ru_{i+1,j+1} = ru_{i-1,j} + (2-2r)u_{i,j} + ru_{i+1,j} \quad \text{(Ia)}

-2\delta t \beta (u_{i,j})(v_{i,j})^2 \quad \text{at } 0 < x < 11, i = 2,3,\ldots,10

\begin{align*}
u_{i,j+1} &= 1 \quad \text{at } x = 1, i = 11

(2 + 2r)v_{1,j+1} - 2rv_{2,j+1} = (2 - 2r - 2\delta t)v_{1,j} + 2rv_{2,j} + 2\delta t (u_{i,j})(v_{i,j})^2 \quad \text{at } x = 0, i = 1 \quad \text{(IIa)}

-rv_{i-1,j+1} + (2+2r)v_{i,j+1} - rv_{i+1,j+1} = rv_{i-1,j} + (2 - 2r - 2\delta t\beta)(v_{i,j}) + rv_{i+1,j} + 2\delta t \beta (u_{i,j})(v_{i,j})^2 \quad \text{at } 0 < x < 11, i = 2,3,\ldots,10

v_{i,j+1} = v_0 \quad \text{at } x = 1 \text{ and } i = 11
\end{align*}

Where \( r = \delta t/\delta x^2 \). Here \( u_{i,j} \) and \( v_{i,j} \) denotes the solution for \( u(x,t) \) and \( v(x,t) \) at space point \( i \) and time iteration \( j \). We use an uniform space-time grid, with space interval \( \delta x \) and time step \( \delta t \).

A method of type (Ia) and (IIa) are known as semi-implicit because the terms on the right-hand side are evaluated partly at the new time step \( j+1 \) and partly at iteration \( j \). such methods were introduced by Crank and Nicolson [2].

4. The Algorithms of the Model

4.1 Explicit Algorithm

Step 1: input a,b,n,m,\( \delta x, \delta t, v_0 \), gamma and beta.

Step 2: set \( r = \delta t/\delta x^2 \) and compute

\( S1 = 1 - 2r, S2 = \delta t/\beta, \text{ and } S3 = S2/\gamma \)

Step 3: set boundary conditions are \( u_{n,1} = 1 \) and \( v_{n,1} = v_0 \) when \( x = 1 \).

Step 4: set the initial conditions are \( u_{i,1} = 1 \) and \( v_{i,1} = v_0 \)

when \( t = 0 \) and \( i = 1,2,\ldots,n \)

Step 5: for \( j = 2,\ldots,m \) and \( i = 1,2,\ldots,n-1 \)

Step 6: if \( i = 1 \) go to step 7 otherwise go to step 8.

Step 7: compute

\( u_{i,j+1} = S1u_{i,j} + 2ru_{2,j} - S2(u_{i,j})(v_{i,j})^2 \text{ and} \)

\( v_{i,j+1} = S1v_{i,j} + 2rv_{2,j} + S2(u_{i,j})(v_{i,j})^2 - S3v_{i,j} \)

Step 8: compute

\( u_{i,j+1} = ru_{i-1,j} + S1u_{i,j} + ru_{i+1,j} - S2(u_{i,j})(v_{i,j})^2 \text{ and} \)

\( v_{i,j+1} = rv_{i-1,j} + S1v_{i,j} + rv_{i+1,j} + S2(u_{i,j})(v_{i,j})^2 - S3v_{i,j} \)

Step 9: end
4.2 Crank-Nicolson Algorithm

Step 1: input a, b, n, m, δx, δt, v₀, gamma and beta.
Step 2: set r = δt/δx² and compute

\[ S_1 = 2 + 2r, \quad S_2 = 2 - 2r, \quad S_3 = \delta t \cdot \text{beta}, \quad \text{and} \quad S_4 = S_3 \cdot \text{gama} \]

Step 3: set boundary conditions \( u_{n,1} = 1 \) and \( v_{n,1} = v_0 \) when \( x = 1 \).
Step 4: set the initial conditions \( u_{i,1} = 1 \) and \( v_{i,1} = v_0 \)
when \( t = 0 \) and \( i = 1, 2, \ldots, n \)
Step 5: solve the tridiagonal linear system \( AX = B \).
Step 6: for \( j = 2, \ldots, m \) and \( i = 1, 2, \ldots, n-1 \)
Step 7: if \( i = 1 \) got to step 8 otherwise go to step 9
Step 8: compute \( v_{b}(i) = S_2 u_{i,j} + 2r u_{i+1,j} - 2S_3 u_{i,j} \)
and \( v_{b1}(i) = (S_2 - 2S_4) v_{i,j} + 2r v_{i+1,j} + 2S_3 u_{i,j} \)
Step 9: compute \( v_{b}(i) = r u_{i-1,j} + S_2 u_{i,j} + r u_{i+1,j} - 2S_3 u_{i,j} \)
and \( v_{b1}(i) = r v_{i-1,j} + (S_2 - 2S_4) v_{i,j} + r v_{i+1,j} + 2S_3 u_{i,j} \)
Step 10: \( u_{i,j} = v_{b}(i), \quad v_{i,j} = v_{b1}(i), \quad i = 1, 2, \ldots, n, \quad j = 1, 2, \ldots, m \).
Step 11: end.

5. Numerical Solutions:

We used the numerical methods to calculate the solution of (2.1) and we take the parameters \( v_0 = 0.1, \gamma = 0.05 \) and \( \beta = 30 \). Since the domain \( 0 < x < 1 \) then we take the step size of space \( \delta x = 0.1 \) and step size of time \( \delta t = 0.005 \) since \( 0 < t < 0.1 \), in this case we get \( r \) less or equal to 0.5 in (I), (II), (Ia) and (II).. The initial conditions of this model are constants but the boundary conditions at \( x=0 \) (i.e. \( i = 1 \)) as a derivative. In this case we see that \( u_{0,j} \) and \( v_{0,j} \) are outside the boundary, thus we use the central-difference approximation to the derivative boundary conditions in order to replace the \( u_{0,j} \) and \( v_{0,j} \) by \( u_{2,j} \) and \( v_{2,j} \) respectively. Then the solution of the numerical results an illustrated by the functions \( u \) and \( v \) of the space \( x \) and time \( t \) in table (1) and table (2) and Figure (1) and (2) for the explicit method and table (3) and table (4) and Figure (3) and (4) for the Crank-Nicolson method.

Table (1): The values of \( u(x_i,t_j) \) using Explicit schemes as \( \delta x=0.1 \) and \( \delta t=0.005 \)

| \( t_i \) | \( x_i \) |
|---|---|
| \( t_0 \) | 0.10000 |
| \( t_1 \) | 0.9985 |
| \( t_2 \) | 0.9970 |
| \( t_3 \) | 0.9955 |
| \( t_4 \) | 0.9939 |
| \( t_5 \) | 0.9923 |

| \( x_i \) | \( x_i=0 \) | \( x_i=0.1 \) | \( x_i=0.2 \) | \( x_i=0.3 \) | \( x_i=0.4 \) | \( x_i=0.5 \) | \( x_i=0.6 \) | \( x_i=0.7 \) | \( x_i=0.8 \) | \( x_i=0.9 \) |
|---|---|---|---|---|---|---|---|---|---|---|
| \( x_i=0 \) | 0.10000 | 0.10000 | 0.10000 | 0.10000 | 0.10000 | 0.10000 | 0.10000 | 0.10000 | 0.10000 | 0.10000 |
| \( x_i=0.1 \) | 0.9985 | 0.9985 | 0.9985 | 0.9985 | 0.9985 | 0.9985 | 0.9985 | 0.9985 | 0.9985 | 0.9985 |
| \( x_i=0.2 \) | 0.9970 | 0.9970 | 0.9970 | 0.9970 | 0.9970 | 0.9970 | 0.9970 | 0.9970 | 0.9970 | 0.9970 |
| \( x_i=0.3 \) | 0.9955 | 0.9955 | 0.9954 | 0.9954 | 0.9954 | 0.9954 | 0.9954 | 0.9954 | 0.9954 | 0.9954 |
| \( x_i=0.4 \) | 0.9939 | 0.9939 | 0.9939 | 0.9939 | 0.9939 | 0.9939 | 0.9939 | 0.9939 | 0.9939 | 0.9939 |
| \( x_i=0.5 \) | 0.9923 | 0.9923 | 0.9923 | 0.9923 | 0.9923 | 0.9923 | 0.9923 | 0.9923 | 0.9923 | 0.9923 |
| \( x_i=0.6 \) | 0.9907 | 0.9907 | 0.9907 | 0.9907 | 0.9907 | 0.9907 | 0.9907 | 0.9907 | 0.9907 | 0.9907 |
| \( x_i=0.7 \) | 0.9891 | 0.9891 | 0.9891 | 0.9891 | 0.9891 | 0.9891 | 0.9891 | 0.9891 | 0.9891 | 0.9891 |
| \( x_i=0.8 \) | 0.9875 | 0.9875 | 0.9875 | 0.9875 | 0.9875 | 0.9875 | 0.9875 | 0.9875 | 0.9875 | 0.9875 |
| \( x_i=0.9 \) | 0.9859 | 0.9859 | 0.9859 | 0.9859 | 0.9859 | 0.9859 | 0.9859 | 0.9859 | 0.9859 | 0.9859 |

46
A Crank-Nicolson Method ...

Table (2): The values of $v(x_i,t_j)$ using Explicit schemes as $\delta x=0.1$ and $\delta t=0.005$

| $x_i$ | $t_j=0$ | $t_j=0.005$ | $t_j=0.010$ | $t_j=0.015$ | $t_j=0.020$ | $t_j=0.025$ | $t_j=0.030$ | $t_j=0.035$ | $t_j=0.040$ | $t_j=0.045$ | $t_j=0.050$ |
|-------|------|---------|---------|---------|---------|---------|---------|---------|---------|---------|---------|
| 0     | 0.1000 | 0.1000  | 0.1000  | 0.1000  | 0.1000  | 0.1000  | 0.1000  | 0.1000  | 0.1000  | 0.1000  | 0.1000  |
| 0.1   | 0.1000 | 0.0997  | 0.0997  | 0.0997  | 0.0997  | 0.0997  | 0.0997  | 0.0997  | 0.0997  | 0.0997  | 0.0997  |
| 0.2   | 0.1000 | 0.0997  | 0.0997  | 0.0997  | 0.0997  | 0.0997  | 0.0997  | 0.0997  | 0.0997  | 0.0997  | 0.0997  |

Table (3): The values of $u(x_i,t_j)$ using Crank-Nicolson schemes as $\delta x=0.1$ and $\delta t=0.005$

| $x_i$ | $t_j=0$ | $t_j=0.005$ | $t_j=0.010$ | $t_j=0.015$ | $t_j=0.020$ | $t_j=0.025$ | $t_j=0.030$ | $t_j=0.035$ | $t_j=0.040$ | $t_j=0.045$ | $t_j=0.050$ |
|-------|------|---------|---------|---------|---------|---------|---------|---------|---------|---------|---------|
| 0     | 1.0000 | 1.0000  | 1.0000  | 1.0000  | 1.0000  | 1.0000  | 1.0000  | 1.0000  | 1.0000  | 1.0000  | 1.0000  |
| 0.1   | 0.9979 | 0.9979  | 0.9979  | 0.9979  | 0.9979  | 0.9979  | 0.9979  | 0.9979  | 0.9979  | 0.9979  | 0.9979  |
| 0.2   | 0.9979 | 0.9979  | 0.9979  | 0.9979  | 0.9979  | 0.9979  | 0.9979  | 0.9979  | 0.9979  | 0.9979  | 0.9979  |

Table (4): The values of $v(x_i,t_j)$ using Crank-Nicolson schemes as $\delta x=0.1$ and $\delta t=0.005$

| $x_i$ | $t_j=0$ | $t_j=0.005$ | $t_j=0.010$ | $t_j=0.015$ | $t_j=0.020$ | $t_j=0.025$ |
|-------|------|---------|---------|---------|---------|---------|
| 0     | 0.1000 | 0.1000  | 0.1000  | 0.1000  | 0.1000  | 0.1000  |
| 0.1   | 0.1000 | 0.1000  | 0.1000  | 0.1000  | 0.1000  | 0.1000  |
| 0.2   | 0.1000 | 0.1000  | 0.1000  | 0.1000  | 0.1000  | 0.1000  |
Table (5) comparison between two numerical methods Explicit and Crank-Nicolson when \( j=11 \) and \( i=1,2,\ldots,11 \).

| Explicit method | Crank-Nicolson method |
|-----------------|-----------------------|
| \( u \) | \( v \) | \( u \) | \( v \) |
| 0.9840 | 0.1082 | 0.9610 | 0.1373 |
| 0.9840 | 0.1082 | 0.9612 | 0.1371 |
| 0.9840 | 0.1082 | 0.9617 | 0.1366 |
| 0.9841 | 0.1082 | 0.9624 | 0.1359 |
| 0.9842 | 0.1081 | 0.9637 | 0.1347 |
| 0.9845 | 0.1080 | 0.9657 | 0.1327 |
| 0.9852 | 0.1076 | 0.9688 | 0.1298 |
| 0.9866 | 0.1069 | 0.9734 | 0.1254 |
| 0.9892 | 0.1056 | 0.9798 | 0.1193 |
| 0.9934 | 0.1034 | 0.9886 | 0.1109 |
| 1.000 | 0.1000 | 1.0000 | 0.1000 |
Figure (1) an illustration of the solution of (2.1) by Explicit method. The solution for $u_{11}$ is plotted as a function space $x$ at successive time $t$, with the parameters $v_0 = 0.1$, $\gamma = 0.05$, $\beta = 30$.

Figure (2) an illustration of the solution of (2.1) by Explicit method. The solution for $v_{11}$ is plotted as a function space $x$ at successive time $t$, with the parameters $v_0 = 0.1$, $\gamma = 0.05$, $\beta = 30$. 
Figure (3) an illustration of the solution of (2.1) by Crank-Nicolson Method. The solution for $u_{11}$ is plotted as a function space $x$ at successive time $t$, with the parameters $v_0 = 0.1, \gamma = 0.05, \beta = 30$.

Figure (4) an illustration of the solution of (2.1) by Crank-Nicolson Method. The solution for $v_{11}$ is plotted as a function space $x$ at successive time $t$, with the parameters $v_0 = 0.1, \gamma = 0.05, \beta = 30$. 

50
6. Conclusion

The system (2.1) of the cubic autocatalytic reaction diffusion was developed by semi-analytical solution. In the semi-analytical model, the governing partial differential equations are by ordinary differential equations. Also this system of reaction diffusion is obtained explicitly by numerical solution. Then we solved this system of reaction diffusion equation numerically with Crank-Nicolson method and we compare it with explicit method, we saw that the Crank-Nicolson method is more accurate than the explicit.
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