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.

طريقة كرانك – نيكولسون لنظم تفاعل ذاتي الانتشار

عباس يونس البياتي سعد عبدالله مناع عبدالغفور محمد امين الروژبياني
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الملخص

في هذا البحث استخدمنا طريقتين عدديتين لحل نظام الانتشار الحراري للمعادلات التفاضلية الجزئية وهما طريقة كرانك – نيكولسون والطريقة الصريحة. للتوضيح طبقنا الطريقتين وقارنا بينهما لحل معادلة انتشار التفاعلات ذات الحافز الذاتي. التي تحتوي على أنتشارين كيميائيين في بعد واحد. واستنتجنا إن النتائج بطريقة كرانك – نيكولسون هي أفضل من النتائج بالطريقة الصريحة.

الكلمات المفتاحية: طريقة كرانك – نيكولسون, الطريقة الصريحة, معادلات تفاعل ذاتي الانتشار.

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

$$u + 2v \rightarrow 3v, \text{ rate} = \beta uv^2, \; v \rightarrow w, \text{ rate} = \beta\gamma v, \qquad (1.1)$$

Where the concentrations of the reactant and autocatalyst are u and v, respectively. The parameters β and γ 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 inter 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:

$$\left.\begin{aligned} &u_t = u_{xx} - \beta uv^2, && (2.1a)\\ &v_t = v_{xx} + \beta uv^2 - \beta\gamma v && (2.1b)\\ &u_x = v_x = 0 \text{ at } x = 0, && (2.1c)\\ &u = 1 \\ &\text{at } x = 1 \text{ and } t = 0 && (2.1d)\\ &v = v_0 \end{aligned}\right\} \quad (2.1)$$

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 β is a measure of the importance of the reaction terms, compared with diffusion, while γ 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

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

and 2.1d is

$u_{i,j} = 1$

at $x = 1$ and $t = 0$

$v_{i,j} = v_0$

thus in general the system (2.1) becomes

$$\left.\begin{aligned} u_{1,j+1} &= (1-2r)u_{1,j}+2ru_{2,j}-\beta\,\delta t\,(u_{1,j})(v_{1,j})^2 \\ &\qquad \text{at } x=0,\ i=1 \\ u_{i,j+1} &= ru_{i-1,j}+(1-2r)u_{i,j}+ru_{i+1,j}-\delta t\beta\,(u_{i,j})(v_{i,j})^2 \\ &\qquad \text{at } 0<x<1,\ i=2,3,\ldots,10 \end{aligned}\right\} \quad \textbf{(I)}$$

$u_{i,j+1} = 1$ at $x = 1$, $i = 11$

$$\left.\begin{aligned} v_{1,j+1} &= (1 - 2r)v_{1,j} + 2rv_{2,j} + \beta\delta t\,(u_{1,j})(v_{1,j})^2 - \beta\delta t\gamma\, v_{1,j} \quad \text{at } x = 0,\ i = 1 \\ v_{i,j+1} &= rv_{i-1,j} + (1 - 2r)\,v_{i,j} + rv_{i+1,j} + \delta t\beta\,(u_{i,j})(v_{i,j})^2 - \delta t\beta\gamma v_{i,j} \quad \text{at } 0 < x < 1,\ i = 2,3,\ldots,10 \\ v_{i,j+1} &= v_0 \quad \text{at } x = 1 \text{ and } i = 11 \end{aligned}\right\} \quad \text{(II)}$$

3.2 The Crank-Nicolson Method:

Thus the Crank-Nicolson method is a simple finite difference method in which a uniform discretisation is used in both space and time, thus from (2.1a) we get:

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

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

$u_{i,j} = 1$

at $x = 1$ and $t = 0$

$v_{i,j} = v_0$

Thus in general the system (2.1) becomes:

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

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

$$u_{i,j+1}=1 \qquad \text{at } x=1,\ i=11$$

$$\left.\begin{aligned}
&(2+2r)v_{1,j+1}-2rv_{2,j+1}=(2-2r-2\beta\delta t)v_{1,j}+2rv_{2,j}+\\
&\qquad 2\beta\delta t\,(u_{1,j})(v_{1,j})^2 \qquad \text{at } x=0,\ i=1\\
&-rv_{i-1,j+1}+(2+2r)v_{i,j+1}-rv_{i+1,j+1}=rv_{i-1,j}+(2-2r-2\delta t\beta\gamma)\,v_{i,j}+\\
&rv_{i+1,j}+2\delta t\beta\,(u_{i,j})(v_{i,j})^2 \qquad \text{at } 0<x<11,\ i=2,3,\ldots,10\\
&v_{i,j+1}=v_0 \qquad \text{at } x=1 \text{ and } i=11
\end{aligned}\right\} \quad \text{(IIa)}$$

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 δx and time step δt.

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,□δx,□δt,v_0, gamma and beta.
Step 2: set $r=\delta t/\delta x^2$and compute
S1 = 1- 2r, S2 = δt.beta and S3 = S2.gama
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,…,n
Step 5: for j = 2,…,m and i = 1,2,…,n-1
Step 6: if i = 1 go to step 7 otherwise go to step 8.
Step 7: compute
$u_{1,j+1}=S1u_{1,j}+2ru_{2,j}-S2\,(u_{1,j})(v_{1,j})^2$ and
$v_{1,j+1}=S1v_{1,j}+2rv_{2,j}+S2\,(u_{1,j})(v_{1,j})^2-S3\,v_{1,j}$

Step 8: compute
$u_{i,j+1}=ru_{i-1,j}+S1u_{i,j}+ru_{i+1,j}-S2\,(u_{i,j})(v_{i,j})^2$and
$v_{i,j+1}=rv_{i-1,j}+S1\,v_{i,j}+rv_{i+1,j}+S2\,(u_{i,j})(v_{i,j})^2-S3\,v_{i,j}$
Step 9: end

4.2 Crank-Nicolson Algorithm

Step 1: input a,b,n,m,□δx,□δt,v_0, gamma and beta.
Step 2: set $r = \delta t/\delta x^2$and compute
S1 = 2 + 2r, S2 = 2 – 2r, S3 = δt.beta and S4 = S3.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,…,n
Step 5: solve the tridiagonl linear system AX = B.
Step 6: for j = 2,…,m and i = 1,2,…,n-1
Step 7: if i = 1 got to step 8 otherwise go to step 9
Step 8: compute $vb(i) = S2u_{i,j} + 2ru_{i+1,j} – 2S3u_{i,j}(v_{i,j})^2$ and
$vb1(i) = (S2 – 2S4)\, v_{i,j} + 2rv_{i+1,j} + 2S3u_{i,j}(v_{i,j})^2$
Step 9: compute $vb(i) = ru_{i-1,j} + S2u_{i,j} + ru_{i+j} – 2S3u_{i,j}\,(v_{i,j})^2$ and
$vb1(i) = rv_{i-1,j} +(S2 – 2S4)\, v_{i,j} + rv_{i+1,j} + 2S3u_{i,j}(v_{i,j})^2$
Step 10: $u_{i,j} = vb(i)$, $v_{i,j} = vb1(i)$, i = 1,2,…,n, j = 1,2,…,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 , γ = 0.05 and β = 30. Since the domain 0 < x < 1 then we take the step size of space δx = 0.1 and step size of time δt= 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 δx=0.1 and δt=0.005

	$x_1 = 0$	x_2=0.1	x_3=0.2	x_4=0.3	x_5=0.4	x_6=0.5	x_7=0.6	x_8=0.7	x_9=0.8	x_{10}=0.9	x_{11}=1
$t_1 = 0$	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000
t_2=0.005	0.9985	0.9985	0.9985	0.9985	0.9985	0.9985	0.9985	0.9985	0.9985	0.9985	1.0000
t_3=0.010	0.9970	0.9970	0.9970	0.9970	0.9970	0.9970	0.9970	0.9970	0.9970	0.9977	1.0000
t_4=0.015	0.9954	0.9954	0.9954	0.9954	0.9954	0.9954	0.9954	0.9954	0.9958	0.9970	1.0000
t_5=0.020	0.9939	0.9939	0.9939	0.9939	0.9939	0.9939	0.9939	0.9941	0.9946	0.9964	1.0000
t_6=0.025	0.9923	0.9923	0.9923	0.9923	0.9923	0.9923	0.9924	0.9927	0.9936	0.9958	1.0000

t_7=0.030	0.9907	0.9907	0.9907	0.9907	0.9907	0.9907	0.9909	0.9914	0.9926	0.9953	1.0000
t_8=0.035	0.9891	0.9891	0.9891	0.9891	0.9891	0.9892	0.9894	0.9901	0.9917	0.9948	1.0000
t_9=0.040	0.9874	0.9874	0.9874	0.9874	0.9875	0.9876	0.9880	0.9890	0.9908	0.9943	1.0000
t_{10}=0.045	0.9857	0.9857	0.9857	0.9857	0.9858	0.9860	0.9866	0.9878	0.9900	0.9938	1.0000
t_{11}= 0.050	0.9840	0.9840	0.9840	0.9841	0.9842	0.9845	0.9852	0.9866	0.9892	0.9934	1.0000

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

	x_1 = 0	x_2=0.1	x_3=0.2	x_4=0.3	x_5=0.4	x_6=0.5	x_7=0.6	x_8=0.7	x_9=0.8	x_{10}=0.9	x_{11}=1
t_1 = 0	0.1000	0.1000	0.1000	0.1000	0.1000	0.1000	0.1000	0.1000	0.1000	0.1000	0.1000
t_2=0.005	0.1008	0.1008	0.1008	0.1008	0.1008	0.1008	0.1008	0.1008	0.1008	0.1008	0.1000
t_3=0.010	0.1015	0.1015	0.1015	0.1015	0.1015	0.1015	0.1015	0.1015	0.1015	0.1011	0.1000
t_4=0.015	0.1023	0.1023	0.1023	0.1023	0.1023	0.1023	0.1023	0.1023	0.1021	0.1015	0.1000
t_5=0.020	0.1031	0.1031	0.1031	0.1031	0.1031	0.1031	0.1031	0.1030	0.1027	0.1018	0.1000
t_6=0.025	0.1039	0.1039	0.1039	0.1039	0.1039	0.1039	0.1039	0.1037	0.1032	0.1021	0.1000
t_7=0.030	0.1047	0.1047	0.1047	0.1047	0.1047	0.1047	0.1046	0.1044	0.1037	0.1024	0.1000
t_8=0.035	0.1056	0.1056	0.1056	0.1056	0.1056	0.1055	0.1054	0.1050	0.1042	0.1027	0.1000
t_9=0.040	0.1064	0.1064	0.1064	0.1064	0.1064	0.1063	0.1061	0.1056	0.1047	0.1029	0.1000
t_{10}=0.045	0.1073	0.1073	0.1073	0.1073	0.1073	0.1071	0.1069	0.1063	0.1051	0.1031	0.1000
t_{11}= 0.050	0.1082	0.1082	0.1082	0.1082	0.1081	0.1080	0.1076	0.1069	0.1056	0.1034	0.1000

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_1 = 0	x_2=0.1	x_3=0.2	x_4=0.3	x_5=0.4	x_6=0.5	x_7=0.6	x_8=0.7	x_9=0.8	x_{10}=0.9	x_{11}=1
t_1 = 0	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000
t_2=0.005	0.9970	0.9970	0.9970	0.9970	0.9970	0.9970	0.9970	0.9971	0.9972	0.9978	1.0000
t_3=0.010	0.9938	0.9938	0.9938	0.9938	0.9938	0.9939	0.9939	0.9942	0.9948	0.9964	1.0000
t_4=0.015	0.9905	0.9905	0.9909	0.9905	0.9905	0.9906	0.9908	0.9914	0.9927	0.9953	1.0000
t_5=0.020	0.9870	0.9870	0.9870	0.9870	0.9871	0.9873	0.9878	0.9888	0.9907	0.9942	1.0000
t_6=0.025	0.9832	0.9832	0.9833	0.9833	0.9835	0.9839	0.9847	0.9862	0.9888	0.9932	1.0000
t_7=0.030	0.9793	0.9793	0.9794	0.9795	0.9798	0.9805	0.9816	0.9836	0.9870	0.9923	1.0000
t_8=0.035	0.9751	0.9751	0.9753	0.9755	0.9760	0.9769	0.9785	0.9811	0.9852	0.9913	1.0000
t_9=0.040	0.9707	0.9708	0.9710	0.9713	0.9721	0.9733	0.9753	0.9786	0.9834	0.9904	1.0000
t_{10}=0.045	0.9660	0.9661	0.9664	0.9670	0.9680	0.9696	0.9721	0.9760	0.9817	0.9895	1.0000
t_{11}= 0.050	0.9610	0.9612	0.9617	0.9624	0.9637	0.9657	0.9688	0.9734	0.9798	0.9886	1.0000

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_1 = 0	x_2=0.1	x_3=0.2	x_4=0.3	x_5=0.4	x_6=0.5	x_7=0.6	x_8=0.7	x_9=0.8	x_{10}=0.9	x_{11}=1
t_1 = 0	0.1000	0.1000	0.1000	0.1000	0.1000	0.1000	0.1000	0.1000	0.1000	0.1000	0.1000
t_2=0.005	0.1029	0.1028	0.1028	0.1028	0.1028	0.1028	0.1028	0.1028	0.1026	0.1021	0.1000
t_3=0.010	0.1059	0.1059	0.1059	0.1059	0.1058	0.1058	0.1058	0.1056	0.1050	0.1034	0.1000
t_4=0.015	0.1090	0.1090	0.1090	0.1090	0.1090	0.1089	0.1087	0.1082	0.1070	0.1045	0.1000
t_5=0.020	0.1124	0.1124	0.1124	0.1124	0.1123	0.1121	0.1116	0.1107	0.1088	0.1055	0.1000

t_6=0.025	0.1160	0.1160	0.1159	0.1159	0.1157	0.1153	0.1146	0.1132	0.1106	0.1065	0.1000
t_7=0.030	0.1198	0.1197	0.1197	0.1195	0.1192	0.1186	0.1175	0.1156	0.1124	0.1074	0.1000
t_8=0.035	0.1238	0.1237	0.1236	0.1234	0.1229	0.1220	0.1205	0.1180	0.1141	0.1083	0.1000
t_9=0.040	0.1280	0.1279	0.1277	0.1274	0.1267	0.1255	0.1235	0.1204	0.1158	0.1091	0.1000
t_{10}=0.045	0.1325	0.1324	0.1321	0.1315	0.1306	0.1291	0.1266	0.1229	0.1175	0.1100	0.1000
t_{11}= 0.050	0.1373	0.1371	0.1366	0.1359	0.1347	0.1327	0.1298	0.1254	0.1193	0.1109	0.1000

Table (5) comparison between two numerical methods Explicit and Crank-Nicolson when j=11 and i=1,2,…,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**

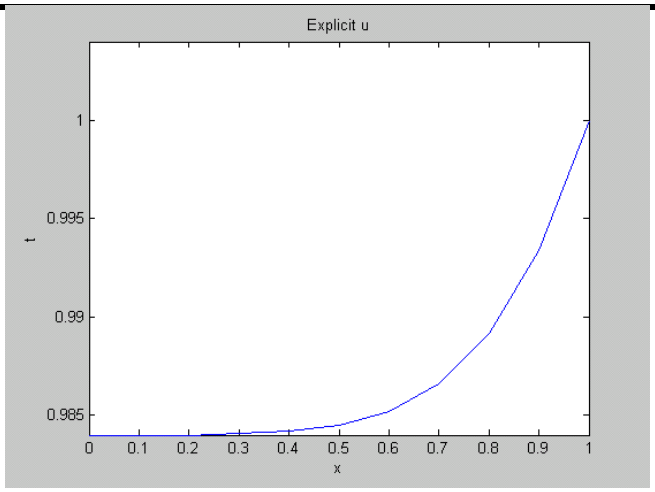

Figure (1) an illustration of the solution of (2.1) by Explicit method. The solution for u_{11} is plotted as a function space x at successive time t, with the parameters
v_0 =0.1 , γ=0.05 , β=30 .

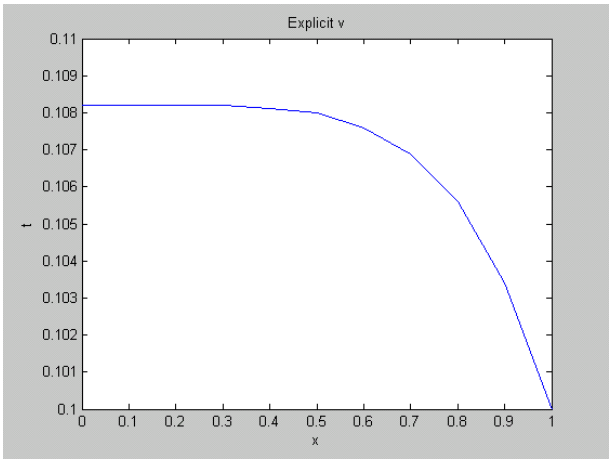

Figure (2) an illustration of the solution of (2.1) by Explicit method. The solution for v_{11} is plotted as a function space x at successive time t, with the parameters v_0 =0.1 , γ=0.05 , β=30 .

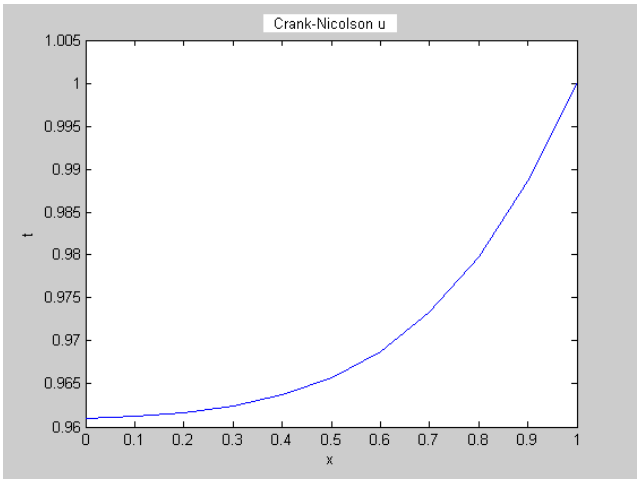

Figure (3) an illustration of the solution of (2.1) by Crank-Nicolson Method. The solution for u_{11} is plotted as a function space x at successive time t, with the parameters
v_0 =0.1 , γ=0.05 , β=30 .

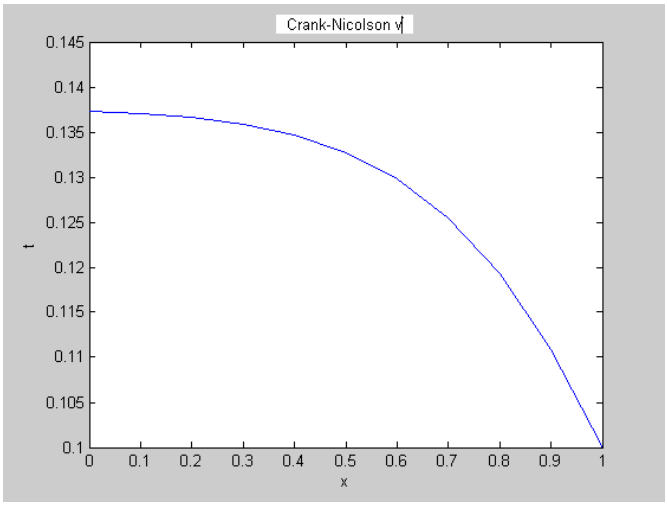

Figure (4) an illustration of the solution of (2.1) by Crank-Nicolson Method. The solution for v_{11} is plotted as a function space x at successive time t, with the parameters v_0 =0.1 , γ=0.05 , β=30 .

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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