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Numerical Solutions of Fractional Order Autocatalytic Chemical Reaction Model

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Abstract: The main concern of this paper is the study and the development of numerical methods for solving fractional order autocatalytic chemical reaction model problem. This is a nonlinear fractional order differential equation of fractional order α, where $0 < \alpha < 1$. Three different (explicit and implicit) schemes based on multistep methods, nonstandard finite difference method and the product integration (PI) method are developed. The first two schemes are based on differential equation model and the PI scheme is constructed by the integral equation formulation of the model problem. The accuracy, efficiency and some numerical comparisons of the developed methods are demonstrated in numerical results.

Kesirli Mertebeden Otokatalitik Reaksiyon Modelinin Nümerik Çözümleri

Anahtar Kelimeler
Kesirli diferansiyel denklemler,
Açık ve Kapalı Yöntemler,
İntegral çarpanı yöntemi,
Standart olmayan yöntem,
Brusselator model

Özet: Bu makale kesirli mertebeden otokatalitik kimyasal modelin nümerik çözümleri ile ilgilidir. Model $0 < \alpha < 1$ için α kesirli mertebeden lineer olmayan bir diferansiyel denklem sistemidir. Çokadımlı yöntemlere dayanan (açık ve kapalı), standart olmayan sonlu fark yöntemi ve integral çarpanı yöntemi (PI) olmak üzere üç farklı nümerik yöntem geliştirilmiştir. İlk iki yöntem diferansiyel denklem modeline ve PI yöntemi model problemin integral denklem formulasyonuna dayanmaktadır. Geliştirilen yöntemlerin tamlığı, etkinliği ve bazı sayısal karşılaştırılmaları nümerik sonuçlarla gösterilmiştir.

1. Introduction

The main concern of this paper is the numerical solution of the autocatalytic chemical reaction (ACR) problem with using the efficient numerical methods.

The ACR problem is mathematically modelled by the following governing equations

$$\begin{cases} {}_cD_{0,t}^{\alpha} x(t) = a-(\mu+1)x(t)+x(t)^2 y(t) \\ {}_cD_{0,t}^{\alpha} y(t) = \mu x(t)-x(t)^2 y(t) \end{cases} \tag{1}$$

where ${}_cD_{0,t}^{\alpha}$ denotes the Caputo's fractional derivative operator, with respect to the origin [34]. The functions $x(t)$ and $y(t)$ are activator and inhibitor variables, respectively, and α, μ are external parameters. The full dynamic of the ACR system is determined by the functions $x(t)$ and $y(t)$ [39].

The fractional order differential equations have been studied extensively in recent years on account of their large significant applications in modeling of various problems in science and engineering. The extension of the concept of fractional order derivative, not only is interesting from theoretical point of view, but also many applied problems are modelled better by this extended tool. An interesting example is the modelling of conservation of mass in fluid dynamics in the case that the control volume is small enough with respect to heterogeneity scale [40]. There are many more other applications such as the field of mechanical systems, dynamical systems, electronic circuit theory, signal processing, control theory, seismology, chaos synchronization that we can extensively use the concept of fractional order derivatives in mathematical modelling of related problems [3, 4, 5, 6, 7, 10, 12, 22, 25, 31, 33, 35, 39]. For more detailed discussion on theoretical and numerical approaches of fractional calculus, especialliy fractional differential equations we refer

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to [29, 32, 34, 36]. The researchers have been developed various schemes for solving fractional differential equations (FDE) in two significant categories: theoretical and numerical approaches. For the sake of completeness we refer to some of them: the nonstandard finite difference method (NSFD) [33], the Adomian decomposition method [30, 31], the variational iteration method [37], the homotopy perturbation method [30], the operational method [23], the differential transform method [1, 13, 14], the Adams-Moulton method [16, 18], the predictor-corrector methods [7, 8, 18] and the product integration rules [20, 38].

The NSFD is one of the our approaches to solve ACR problem in this paper. This scheme was firstly proposed by Mickens for solving ordinary differential equations and following that many reserchers made many developments and extended it to FDEs, see for instance [26, 27, 28].

In this paper, we present implicit and explicit schemes for solving ACR problem (1) based on three methodologies [2]: the first two approaches are based on the original differential equation (1) and the third method is based on the integral equation (IE) reformulation of ACR model problem. The ACR model is equivalently modeled by a Voltera integral equation of the second kind, in which we can produce both explicit and implicit schemes using the product integration (PI) method. In summary, these methodologies provide three implicit and explicit methods based on multistep, NSFD and PI methods. The organization of this paper is as follow: In section 2, we shortly review the preliminaries and required notations from fractional calculus. In section 3, we derive the different numerical approaches for ACR model problem (1). More precisley, we develop the following schemes, respectively:

1. The explicit and implicit multistep methods
2. The explicit and implicit product integration methods
3. The explicit and implicit NSFD schemes

Finally, in section 4, we present the numerical results with a detailed comparision of the methods.

2. Introductory Material

This section provides a brief review of the necessary concepts and some of the main definitions from fractional calculus. There are several ways to introduce the notion of fractional derivative. Accordingly, the basic step in solving a fractional differential equation is to find a way to approximate the corresponding fractional order derivatives. Let $\alpha > 0$ be an arbitrary real number and $m = [\alpha]$ is the smallest integer such that $m > \alpha$. The Caputo's derivative of fractional order α is defined by

$$ {}_{c}D_{0,t}^{\alpha}u(t) = \frac{1}{\Gamma(m-\alpha)}\int_0^t (t-\tau)^{m-1-\alpha}u^{(m)}(\tau)d\tau. \quad (2)$$

On the other hand, the historically worthwhile definition of the Riemann-Liouville (RL) fractional derivative of order α is as follow:

$$ {}_{RL}D_t^{\alpha}u(t) = \frac{1}{\Gamma(m-\alpha)}\frac{d^m}{dt^m}\int_0^t (t-\tau)^{m-1-\alpha}u(\tau)d\tau. \quad (3)$$

There is a close relation between Caputo's derivative in the sense that if $g(t)$ is the α -order derivative of $u(t)$, i.e.,

$$ {}_{c}D_{0,t}^{\alpha}u(t) = g(t), \quad (4)$$

then we have

$$ u(t) = U_{m-1}(t) + {}_{RL}D_t^{\alpha}g(t), \quad (5)$$

where $U_{m-1}(t)$ is the Taylor polynomial of degree $m-1$ about the origin

$$ U_{m-1}(t) = \sum_{k=0}^{m-1}\frac{t^k}{k!}u^{(k)}(0). \quad (6)$$

The inverse relation is also holds in the following sense

$$ g(t) = {}_{RL}D_t^{-\alpha}(u(t) - U_{m-1}(t)). \quad (7)$$

The practical alternative is the Grunwald-Letnikov (GL) operator

$$ {}^{GL}D_t^{\alpha}y(t) = \lim_{N\to\infty}\frac{1}{h^{\alpha}}\sum_{k=0}^{N}\omega_k^{(\alpha)}y(t-kh), \quad (8)$$

where $t\epsilon(t_0, t]$, and $h = \frac{t}{N}$ depends on t and N. The weights w_j^{α} are the coefficients of power series expansion of $(1-\xi)^{\alpha}$, i.e.,

$$ \omega_j^{(\alpha)} = (-1)^j\binom{\alpha}{j} = \frac{\Gamma(j-\alpha)}{\Gamma(-\alpha)\Gamma(j+1)}$$

Throughout the paper we shall regularly be using the following notations;

$$ \bar{x}_{n-1} = \begin{cases} \omega_n^{(\alpha-1)}x_0 & n = 1 \\ \omega_n^{(\alpha-1)}x_0 - \sum_{j=2}^{n}\omega_j^{(\alpha)}x_{n-j} & n \geq 2, \end{cases}$$

the same notation also holds for $\bar{y}_{n-1}$. Accordingly, the weights $\omega_j^{(\alpha)}$, that are the coefficients of the power series expansion, can be written as follow

$$\begin{cases} \omega_n^{(\alpha-1)} x_0 - X_n = \bar{x}_{n-1} + \alpha x_{n-1} \\ \omega_n^{(\alpha-1)} y_0 - Y_n = \bar{y}_{n-1} + \alpha y_{n-1}, \end{cases}$$

where

$$X_n = \sum_{j=1}^{n} \omega_j^{(\alpha)} \bar{x}_{n-j}, \quad Y_n = \sum_{j=1}^{n} \omega_j^{(\alpha)} \bar{y}_{n-j}.$$

3. Numerical Schemes

This section deals with the development of explicit and implicit numerical methods for solving ACR model problem (1). In implicit schemes we the reduced nonlinear system of equations are handled by Newton-Raphson method.

3.1. Explicit and implicit multistep methods

The linear multistep methods such as Adams-Moulton methods have been studied in detail by Garrappa and Galeone in a series of papers [15, 16, 17, 18]. To develop the idea to the ACR problem (1) we first propose the following general fractional differential equation (FODE),

$$D^{\alpha} y(t) = f(t, y(t)), \tag{9}$$

where $y: [t_0, T] \longrightarrow \mathbb{R}^q$ is an unknown function and $f: [t_0 T] \times \mathbb{R}^q \longrightarrow \mathbb{R}^q$ is a sufficiently smooth function. Without losing generality, we propose the scalar case $q = 1$, it is straightforward to extend the presented methods for the general system of FODE. Let us consider the FODE (9) at the grid points $t = t_{n-1}$

$$D^{\alpha} y(t_n) = f(t_{n-1}, y(t_{n-1})), \tag{10}$$

where $f(t_{n-1}, y(t_{n-1})) = f(t_{n-1}, y_{n-1}) = f_{n-1}$. To obtain a fully discrete scheme it is required to find an approximate value of $D^{\alpha} y(t_{n-1})$ in terms of point values of the unknown function y . To accomplish this we use the GL operator (8) as an approximation of $D^{\alpha} y(t_{n-1})$. Therefore, using the GL operator (8) the FODE model (10) can be written as follow

$${}_{a}^{GL}D_t^{\alpha} f(t_{n-1}) = f(t_{n-1}, y(t_{n-1})),$$

or

$$h^{-\alpha} \sum_{j=0}^{n} \omega_j^{\alpha} (y_{n-j} - y_0) = f(t_{n-1}, y(t_{n-1})),$$

or equivalently,

$$\sum_{j=0}^{n-1} \omega_j^{\alpha} y_{n-j} - y_0 \sum_{j=0}^{n-1} \omega_j^{\alpha} = h^{\alpha} f(t_{n-1}, y(t_{n-1})).$$

There is an explicit representation for $b_n = \sum_{j=0}^{n-1} \omega_j^{\alpha}$ as follows [14, 15, 16],

$$b_n = \frac{-\alpha \Gamma(n-\alpha)}{\Gamma(2-\alpha)\Gamma(n-1)}, \quad n \geq 1,$$

therefore, we have

$$y_0 \omega_0 + \sum_{j=1}^{n-1} \omega_j^{\alpha} y_{n-j} - y_0 b_n = h^{\alpha} f(t_{n-1}, y(t_{n-1})).$$

finally the explicit scheme reduces as follow

$$y_n = h^{\alpha} f(t_{n-1}, y(t_{n-1})) - \sum_{j=1}^{n-1} \omega_j^{\alpha} y_{n-j} - y_0 b_n. \tag{11}$$

Now, the explicit method for ACR model (1) reads

$$\begin{cases} x_n = \bar{x}_{n-1} + \alpha x_{n-1} + h^{\alpha} [a - (\mu+1) x_{n-1} + x_{n-1}^2 y_{n-1}], \\ y_n = \bar{y}_{n-1} + \alpha y_{n-1} + h^{\alpha} [\mu x_{n-1} + x_{n-1}^2 y_{n-1}]. \end{cases} \tag{12}$$

The implicit variant is similarly drived by considering the FODE (10) at the grid point $t = t_{n-1}$. Therefore, using the truncated GL operator for fractional derivative we obtain

$$h^{-\alpha} \sum_{j=0}^{n} \omega_j^{\alpha} (y_{n-j} - y_0) = f(t_n, y(t_n)),$$

it turns out that

$$y_n - h^{\alpha} f(t_n, y(t_n)) = y_0 b_n - \sum_{j=1}^{n-1} \omega_j^{\alpha} y_{n-j}. \tag{13}$$

The equation (13) is implicit in y_n and we need a nonlinear system solver to find the unknown value y_n To accomplish this we use the Newton-Raphson method with the following iteration function

$$g(z) = z - h^{\alpha} f(t_n, z) - y_0 b_n + \sum_{j=1}^{n-1} \omega_j^{\alpha} y_{n-j},$$

and

$$g'(z) = 1 - h^{\alpha} f'(t_n, z),$$

then, the recursive relation to obtain y_n is written as follow

$$z_{i+1} = z_i - \frac{g(z_i)}{g'(z_i)}, \quad i = 0,1, \dots ,$$

where the initial guess is $z_0 = y_{n-1}$. Therefore, the iterations for solving ACR problem (1) reads

$$\begin{cases} z_{i+1} = z_i - \dfrac{z_i + \sum_{j=1}^{n-1}\omega_j^{(\alpha)} x_{n-j} - \omega_n^{(\alpha-1)} x_0 - h^\alpha[a-(\mu+1)z_i + z_i^2 y_n]}{1+(\mu+1)h^\alpha + 2z_i y_n}, \\ y_n = \dfrac{h^\alpha \mu x_n - \sum_{j=1}^{n-1}\omega_j^{(\alpha)} y_{n-j} + \omega_n^{(\alpha-1)} y_0}{1-h^\alpha x_n^2}. \end{cases} \quad (14)$$

3.2. Product integration method

In this section we use the reformulation of the ACR problem as a Volteral integral equation (VIE). Then we propose the numerical solution of the reduced VIE with product integration method.

The corresponding VIE formulation of ACR problem is [21]

$$y(t) = y(t_0) + \frac{1}{\Gamma(\alpha)}\int_{t_0}^{t}(t-s)^{\alpha-1} f(s, y(s))ds. \quad (15)$$

this is a convolution type integral equation and the product integration approach can be applied efficiently for this problem [20, 38]. For further study of the more recent approaches for solving FDEs based on product integration we refer to [8, 19, 20, 23]. We consider a uniform grid $t_j = t_0 + jh$, where h is grid spacing and we consider the piecewise constant approximation $f(s, y(s)) \approx f_j = f(t_j, y(t_j))$ for all $s \in [t_j, t_{j+1}]$. Then, the explicit product integration method is given by

$$y(t_n) = y_0 + \frac{1}{\Gamma(\alpha)}\sum_{j=0}^{n-1} f_j \int_{t_j}^{t_{j+1}}(t_n - s)^{\alpha-1} ds, \quad (16)$$

where we have

$$\int_{t_j}^{t_{j+1}}(t_n - s)^{\alpha-1}ds = \int_{t_j}^{t_n}(t_n - s)^{\alpha-1}ds + \int_{t_n}^{t_{j+1}}(t_n - s)^{\alpha-1}ds$$
$$= \frac{h^\alpha}{\alpha}((n-j)^\alpha - (n-j-1)^\alpha), \quad (17)$$

substituting (17) in (16) we obtain

$$y_n = y_0 + \frac{1}{\Gamma(\alpha+1)}\sum_{j=0}^{n-1} h^\alpha f_j((n-j)^\alpha - (n-j-1)^\alpha). \quad (18)$$

On defining

$$b_{n-j-1} = \frac{(n-j)^\alpha - (n-j-1)^\alpha}{\Gamma(\alpha+1)},$$

we can rewrite (18) as follow

$$y_n = y_0 + h^\alpha \sum_{j=0}^{n-1} b_{n-j-1} f_j. \quad (19)$$

Now, the application of this scheme for ACR model (1) results as follow

$$\begin{cases} x_n = x_0 + h^\alpha \sum_{j=0}^{n-1} b_{n-j-1}[a-(\mu+1)x_j + x_j^2 y_j], \\ y_n = y_0 + h^\alpha \sum_{j=0}^{n-1} b_{n-j-1}[\mu x_j + x_j^2 y_j]. \end{cases} \quad (20)$$

Similarly, the application of the implicit product integration for (1) reduces to the following equations

$$\begin{cases} x_n = x_0 + h^\alpha f_0 d_{n,0} + h^\alpha \sum_{j=1}^{n} a_{n-j} f_j, \\ y_n = y_0 + h^\alpha g_0 d_{n,0} + h^\alpha \sum_{j=1}^{n} a_{n-j} g_j, \end{cases} \quad (21)$$

where the coefficients $d_{n,0}$ and a_n are

$$d_{n,0} = \frac{(n-1)^{\alpha+1} - n^\alpha(n-\alpha-1)}{\Gamma(\alpha+2)},$$

and

$$a_n = \begin{cases} \dfrac{1}{\Gamma(\alpha+2)}, & n = 0 \\ \dfrac{(n-1)^{\alpha+1} - 2n^{\alpha+1} + (n+1)^{\alpha+1}}{\Gamma(\alpha+2)} & n = 1,2, \dots . \end{cases}$$

3.3. Explicit and implicit nonstandard finite difference methods

Now, we develop the implicit and explicit nonstandard finite difference schemes.

Following [33], we resolve the nonlinear terms of ACR model (1) in the following sort

$$\begin{cases} x(t) \to x(t_{n-1}), \\ x^2(t)y(t) \to x(t_n)x(t_{n-1})y(t_{n-1}). \end{cases}$$

Taking into account these sunstitutions and applying the truncated GL operator, we find the following fully discrete equations

$$\begin{cases} x_n+\sum_{j=1}^{n}\omega_j^{(\alpha)}x_{n-j}-\omega_n^{(\alpha-1)}x_0=\phi(h)[a-(\mu+1)x_{n-1}+x_nx_{n-1}y_{n-1}], \\ y_n+\sum_{j=1}^{n}\omega_j^{(\alpha)}y_{n-j}-\omega_n^{(\alpha-1)}y_0=\phi(h)[\mu x_{n-1}+x_nx_{n-1}y_{n-1}], \end{cases}$$

this means that, we can explicitly evaluate x_n and y_n as follow

$$\begin{cases} x_n=\dfrac{\omega_n^{(p-1)}x_0-\sum_{j=1}^{n}\omega_j^{(\alpha)}x_{n-j}+\phi(h)[a-(\mu+1)x_{n-1}]}{1-\phi(h)x_{n-1}y_{n-1}}, \\ y_n=\omega_n^{(\alpha-1)}y_0-\sum_{j=1}^{n}\omega_j^{(p)}y_{n-j}+\phi(h)[\mu x_{n-1}+x_nx_{n-1}y_{n-1}], \end{cases}$$

or,

$$\begin{cases} x_n=\dfrac{\overline{x}_{n-1}+x_{n-1}(\alpha-\phi(h)(\mu+1))+a\phi(h)}{1-\phi(h)x_{n-1}y_{n-1}}, \\ y_n=\overline{y}_{n-1}+y_{n-1}(\alpha+\phi(h))x_nx_{n-1})+\phi(h)\mu x_{n-1}. \end{cases} \quad (22)$$

The implicit discretization is accomplished with the following modifications

$$\begin{cases} x(t)\rightarrow x(t_n), \\ x^2(t)y(t)\rightarrow x(t_n)x(t_n)y(t_n). \end{cases}$$

inserting these substitutions in the ACR model (1) and using the truncated GL operator we obtain

$$\begin{cases} \sum_{j=1}^{n}\omega_j^{(\alpha)}(x_{n-j}-x_0)=\phi(h)[a-(\mu+1)x_n+x_nx_ny_n], \\ \sum_{j=1}^{n}\omega_j^{(\alpha)}(y_{n-j}-y_0)=\phi(h)[\mu x_n+x_nx_ny_n], \end{cases} \quad (23)$$

In this case, (23) is a nonlinear systems in terms of x_n, therefore, we have to invoke an appropriate nonlinear systems solver to obtain the unknowns. To accomplish this we use Newton-Raphson method with the following iteration function

$$\begin{cases} g(z)=z+\sum_{j=1}^{n-1}\omega_j^{(\alpha)}x_{n-j}-\omega_n^{(p-1)}x_0-\phi(h)[a-(\mu+1)z+x_nz^2y_n], \\ y_n=\dfrac{\phi(h)\mu x_n-\sum_{j=1}^{n-1}\omega_j^{(\alpha)}y_{n-j}+\omega_n^{(p-1)}y_0}{1-\phi(h)x_nx_n}, \end{cases}$$

The Newton-Raphson iterations $z_{i+1}=z_i-\dfrac{g(z_i)}{g'(z_i)}, i=0,1,\ldots$ will converge to x_n with initial guess $z_0=x_{n-1}$. In the test problems we use the following denominator function $\phi(h,\mu+1)=\dfrac{1-e^{-h^{\alpha}(\mu+1)}}{\mu+1}$. And as an alternative we can use $(\dfrac{1-e^{-h(\mu+1)}}{\mu+1})^p$, which is proposed by some authors [26, 27, 28, 33].

4. Results

In this section we demonstrate the numerical results for ACR model problem (1) with using specific parameters and grid spacing. The computations are carried out at prescribed parameters $a=1, \mu=2, p=0.8$, in the time interval [0,50] with grid spacing $h=0.05$ and the initial data $(x_0,y_0)=(0.9,2.1)$.

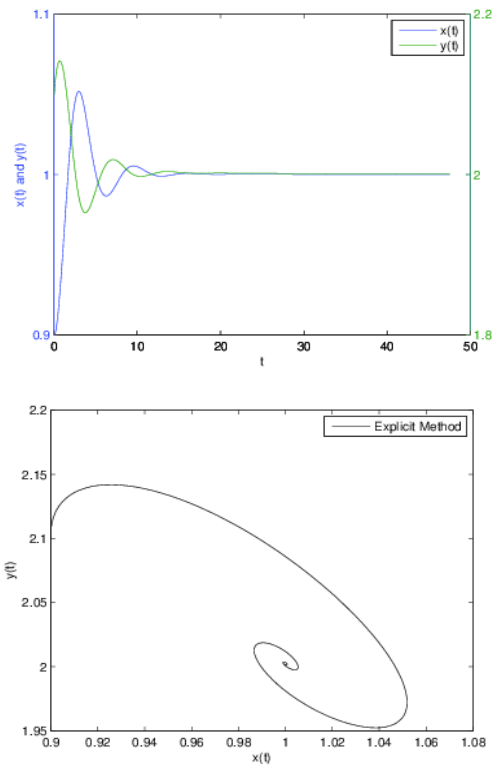

Figure 1: Numerical results with explicit multistep method (12).

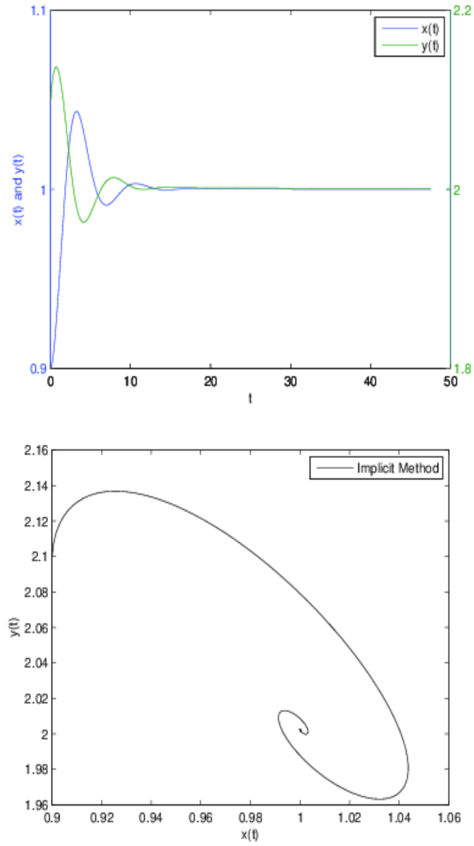

Figure 2: Numerical results with implicit multistep method (13).

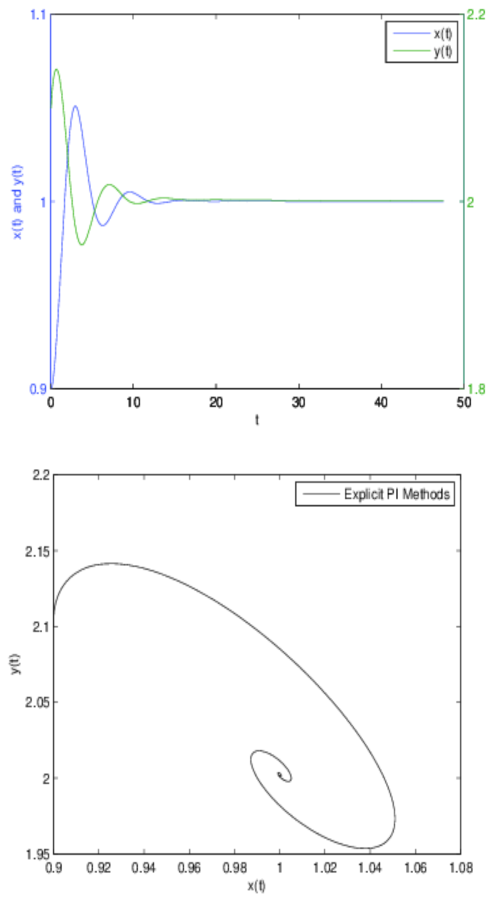

Figure 3: Numerical results with explicit PI method (20).

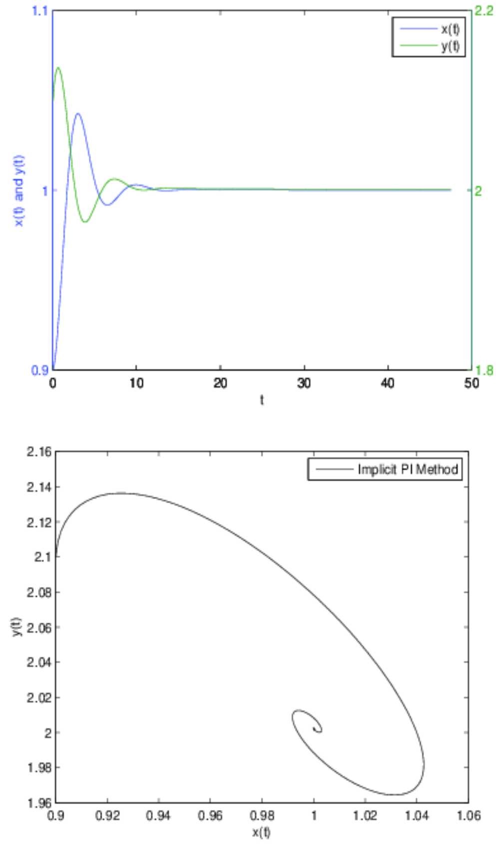

Figure 4: Numerical results with implicit PI method (21).

The numerical results are illustrated in $(t, x(t))$ plane for both $x(t)$ and $y(t)$, and the solution in the phase plane is also provided in the figures.

In Figure 1 the numerical results of explicit multistep method (12) are shown for problem (1). In the left portion the graphs $x(t)$ and $y(t)$ are demonstrated versus the time variable t and the right portion shows the corresponding numerical results in phase plane. Recalling the theoretical behavior of the model problem (1) we find that the numerical results of the explicit scheme (12) are stable. Figure 2 illustrates the same results for implicit multistep method (13). Figure 3, similarly, demonstrates the results for explicit PI method (20). Figure 4 shows the results for implicit PI method (21). Figure 5 represents the numerical results for explicit NSFD method (22). Figure 6, finally, is the graph of the numerical results in the case of implicit NSFD method (23). All the simulations with the derived schemes illustrate the stable behavior of the general solution.

5. Discussion and Conclusion

We have developed three different explicit and implicit schemes for solving ACR problem (1). The multistep, nonstandard finite difference and product integration methods. These methods introduced in explicit and implicit modes. According to the numerical results and their comparison, the presented schemes are accurate and also they have stable behavior in simulating the true solution.

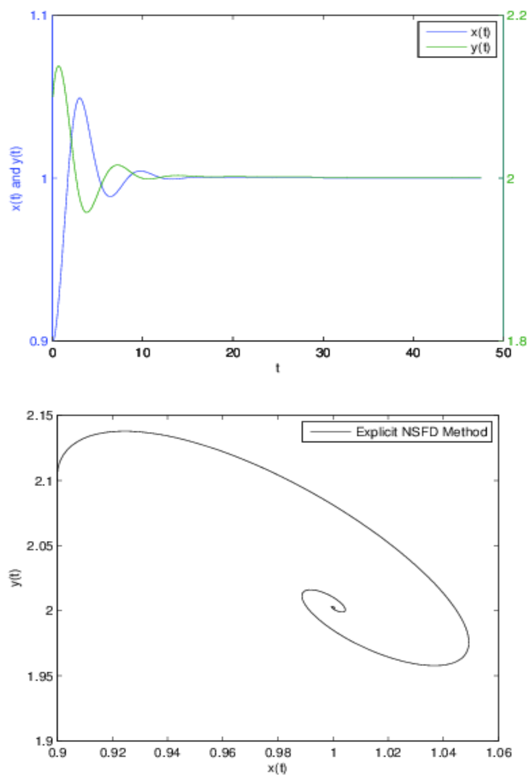

Figure 5: Numerical results with explicit NSFD method (22).

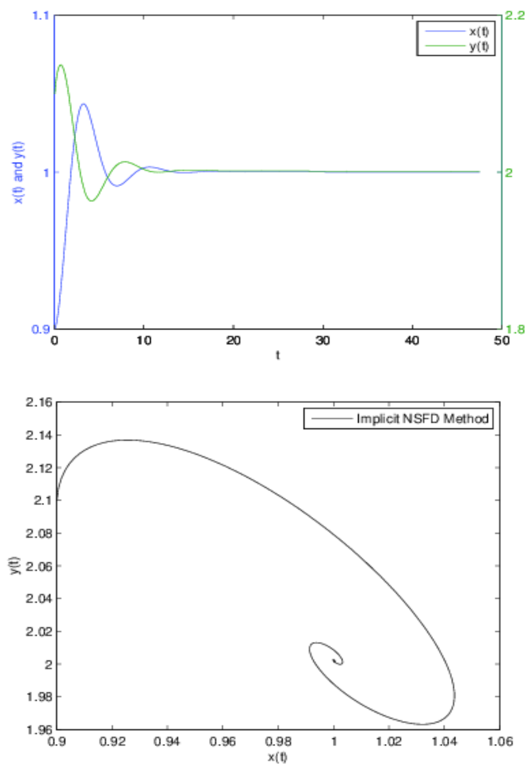

Figure 6: Numerical results with implicit NSFD method (23).

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