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Efficient Explicit Nonstandard Finite Difference Scheme with Positivity-Preserving Property

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Abstract

Parabolic equations in which advection-diffusion transports are coupled to reactions terms arise in different science and engineering fields, including physical and biological systems. Usually, in practical applications the unknowns are concentration of chemical compounds or population sizes being positive also from their physical nature as well. Widely used schemes such as classical finite difference may produce numerical drawbacks such as spurious oscillations and negative values in the solution because of truncation errors and may then become unstable. By using the nonstandard finite difference (NSFD) method, a better finite difference model is constructed. The proposed NSFD scheme, guarantees the positivity of the solutions and returns spurious oscillations free, solutions.

1. INTRODUCTION

In order to solve advection-diffusion reaction equation, analytical and numerical solution techniques are used. Analytical solution of this equation may be carried out when simple and idealized conditions are satisfied. However, if the solution parameters change in time, use of the numerical solution techniques is necessary for the solution of advection-diffusion reaction equation. It is desirable that the numerical solutions satisfy the same properties as the exact solution such as positivity, total variation dimensioning or monotonicity [4, 8, 11, 12]. The standard advection-diffusion reaction model deals with the physical and biological phenomena such as heat transfer, transport, reaction of chemical species, population density in biology and adsorption of pollutants in soil [1, 3, 20, 21]. In these cases, the components of the unknown can denote concentrations of chemical species, population sizes which are quantities and they need to remain positive, so we need to develop numerical techniques that preserve the positivity of solution. One of the shortcomings of the standard finite difference method is that the above mentioned qualitative properties of the exact solution usually are not transferred to the numerical solution. Furthermore, many problems may affect the stability properties of the standard approach. One way of avoiding this disadvantage is to imply finite difference schemes that are nonstandard in the sense of Mickens' definition [15]. The present work which is motivated by many successful papers on the matter [2, 9, 10, 13, 14, 16, 17, 18, 19], introduces a family of NSFD schemes to approximate consistent solutions of the standard advection-diffusion reaction equations, which is an equation for which the existence of non-negative solutions is a well-known fact. The proposed methods satisfy property of positivity, and they are stable for appropriate choice of the model parameter.

The rest of the paper is organized as follows: In Section 2, we propose the new method and investigate the positivity and stability requirements. In Section 3, we apply the method to four problems and compared with standard finite difference schemes. Finally, we end the paper with some conclusions in Section 4.

2. SCHEME CONSTRUCTION

Consider the standard advection-diffusion reaction equation

$$\frac{\partial C(x,t)}{\partial t} + P\frac{\partial C(x,t)}{\partial x} - Q\frac{\partial^2 C(x,t)}{\partial x^2} = -RC, \qquad (x,t) \in [0, x_{\max}] \times [0,T], \tag{1}$$

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where $C_j^n \simeq C\left(x_j, t_n\right)$, and the solution domain of the problem is covered by a mesh of grid-lines $x_j = j\Delta x$ and $t_n = n\Delta t$, such that $j = 0,1,2,\cdots,M$ an $n = 0,1,2,\cdots,N$, where x_j and t_n are parallel to the space and time coordinate axes. The constant spatial and temporal grid spacing are $\Delta x = \frac{x_{\max}}{M}$ and $\Delta t = \frac{T}{N}$.

In order to derive an accurate NSFD scheme for (1) which is positivity preserving, we replace the reaction term in (1) by

$$a\left(C_{j+1}^n + C_{j-1}^n\right) + \left(1-2a\right)C_j^{n+1}, \tag{2}$$

here a is arbitrary parameter to be determined below. Therefore, by using the central second order finite difference approximation schemes for the spatial operators (first and second order derivatives), the discretization of (1) can be considered as:

$$\left(\frac{1}{\Delta t} + \left(1-2a\right)R\right)C^{n+1} = AC^n, \tag{3}$$

where C^n is the transpose of vector $\left[C_0^n, C_1^n, \cdots, C_M^n\right]$ and A is the following tridiagonal matrix

$$A = tridiag\left\{\frac{P}{2\Delta x} + \frac{Q}{\Delta x^2} - Ra; \frac{1}{\Delta x} - \frac{2Q}{\Delta x^2}; -\frac{P}{2\Delta x} + \frac{Q}{\Delta x^2} - Ra\right\}. \tag{4}$$

The parameter a is chosen according to the following theorem:

Theorem 1. Sufficient for scheme (3) to be positive is,

$$a \le \frac{\frac{Q}{\Delta x^2} - \frac{P}{2\Delta x}}{R} \quad , \quad \Delta t \le \frac{\Delta x^2}{2Q}. \tag{5}$$

Proof. From (3) it is enough to show that $A \ge 0$, then we have to put

$$\frac{P}{2\Delta x} + \frac{Q}{\Delta x^2} - Ra \ge 0, \tag{6}$$

$$-\frac{P}{2\Delta x} + \frac{Q}{\Delta x^2} - Ra \ge 0, \tag{7}$$

$$\frac{1}{\Delta x} - \frac{2Q}{\Delta x^2} \ge 0, \tag{8}$$

from (6) and (7), we have $a \le \frac{\frac{Q}{\Delta x^2} - \frac{P}{2\Delta x}}{R}$ and from (8), we can derive $\Delta t \le \frac{\Delta x^2}{2Q}$, with conditions (5), we have $\frac{1}{\Delta t} + \left(1-2a\right)R \ge 0$, then the solution is positive.

Theorem 2. The new scheme is conditionally stable and convergent with local truncation error $O\left(\Delta t, \Delta x^2\right)$.

Proof. Under condition (5), we have $\frac{1}{\frac{1}{\Delta t} + \left(1-2a\right)R} \ge 0$. In the other hand we have $\| A \|_\infty = \frac{1}{\Delta t} - 2Ra$, and for spectral radius, ρ of the iteration matrix we derive

$$\rho\left(\left[\frac{1}{\frac{1}{\Delta t}+(1-2a)R}\right]A\right)\leq\|\left[\frac{1}{\frac{1}{\Delta t}+(1-2a)R}\right]A\|_{\infty}\leq|\frac{1}{\frac{1}{\Delta t}+(1-2a)R}|\,\|A\|_{\infty}\leq\frac{\frac{1}{\Delta t}-2Ra}{\frac{1}{\Delta t}-2Ra+R}<1, \tag{9}$$

therefore the scheme is stable and then via the Lax-theorem [22] convergent with local truncation error:

$$\begin{aligned}T_j^n=&\frac{C(x_j,t_{n+1})-C(x_j,t_n)}{\Delta t}+P\frac{C(x_{j+1},t_n)-C(x_{j-1},t_n)}{2\Delta x}\\&-Q\frac{C(x_{j-1},t_n)-2C(x_j,t_n)+C(x_{j+1},t_n)}{\Delta x^2}\\&+R\Big(a\big(C(x_{j+1},t_n)+C(x_{j-1},t_n)\big)+(1-2a)C(x_j,t_{n+1})\Big),\end{aligned} \tag{10}$$

by Taylor's expansion

$$C(x_j,t_{n+1})=C(x_j,t_n)+\Delta t\left(\frac{\partial C}{\partial t}\right)(x_j,t_n)+\frac{1}{2}\Delta t^2\left(\frac{\partial^2 C}{\partial t^2}\right)(x_j,t_n)+\frac{1}{6}\Delta t^3\left(\frac{\partial^3 C}{\partial t^3}\right)(x_j,t_n)+\cdots,$$

$$C(x_{j+1},t_n)=C(x_j,t_n)+\Delta x\left(\frac{\partial C}{\partial x}\right)(x_j,t_n)+\frac{1}{2}\Delta x^2\left(\frac{\partial^2 C}{\partial x^2}\right)(x_j,t_n)+\frac{1}{6}\Delta x^3\left(\frac{\partial^3 C}{\partial x^3}\right)(x_j,t_n)+\cdots,$$

$$C(x_{j+1},t_n)=C(x_j,t_n)-\Delta x\left(\frac{\partial C}{\partial x}\right)(x_j,t_n)+\frac{1}{2}\Delta x^2\left(\frac{\partial^2 C}{\partial x^2}\right)(x_j,t_n)-\frac{1}{6}\Delta x^3\left(\frac{\partial^3 C}{\partial x^3}\right)(x_j,t_n)+\cdots,$$

by substitution into (10) we have

$$\begin{aligned}T_j^n=&\left(\frac{\partial C}{\partial t}+P\frac{\partial C}{\partial x}-Q\frac{\partial^2 C}{\partial x^2}+RC\right)(x_j,t_n)\\&+R(1-2a)\Delta t\left(\frac{\partial C}{\partial t}\right)(x_j,t_n)+\frac{1}{2}\Delta t\left(\frac{\partial^2 C}{\partial t^2}\right)(x_j,t_n)+Ra\Delta x^2\left(\frac{\partial^2 C}{\partial x^2}\right)(x_j,t_n)+\cdots,\end{aligned} \tag{11}$$

hence the scheme is consistent with (1) and $T_j^n=O\left(\Delta t,\Delta x^2\right)$.

3. NUMERICAL SIMULATIONS

To test the proposed method with respect to positivity and stability, developed in previous section, we have integrated several problems of different applications nature. We validate the method by comparing it to exact solutions and also with solutions obtained from the other methods.

3.1. Example 1: Exponential traveling wave

The first example consists of equation (1) for $P=1$, $Q=1$ and $R=1$:

$$\frac{\partial C(x,t)}{\partial t}+\frac{\partial C(x,t)}{\partial x}-\frac{\partial^2 C(x,t)}{\partial x^2}=-C(x,t),\qquad (x,t)\in[0,x_{\max}]\times[0,T], \tag{12}$$

with initial condition:

$$C(x,0)=\exp(-x),\qquad x\in[0,x_{\max}], \tag{13}$$

and boundary conditions:

$$\begin{aligned} &C(0,t) = \exp(t), \qquad t \in [0,T], \\ &\frac{\partial C(x_{\max},t)}{\partial x} = -C(x_{\max},t), \qquad t \in [0,T]. \end{aligned} \tag{14}$$

The exact solution is given by

$$C(x,t) = \exp(t-x) \tag{15}$$

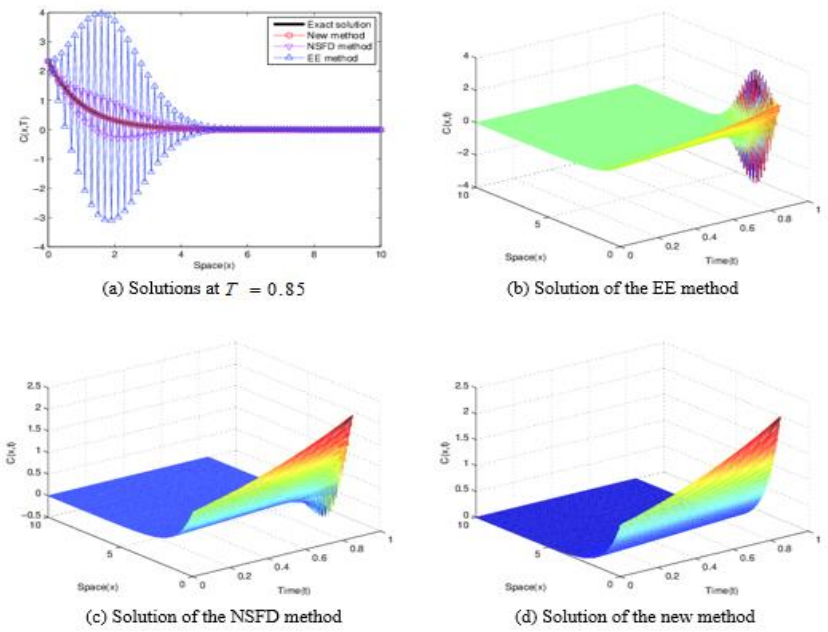
In order to show the advantages of the proposed new method, we numerically solve (12) for $x_{\max} = 10$ and $T = 0.85$ using $\Delta x = 0.1$ and $\Delta t = 0.005$. In addition to comparing the solution of the new scheme with the exact solution, we also compare it to the numerical solution produced by a standard upwind forward Euler finite difference method (EE):

$$\frac{C_j^{n+1} - C_j^n}{\Delta t} + \frac{C_j^n - C_{j-1}^n}{\Delta x} - \frac{C_{j-1}^n - 2C_j^n + C_{j+1}^n}{\Delta x^2} = -C_j^n, \tag{16}$$

and the nonstandard finite-difference (NSFD) method, proposed by Mickens in [16]:

$$\frac{C_j^{n+1} - C_j^n}{\Delta t} + \frac{C_j^n - C_{j-1}^n}{\Delta x} - \frac{C_{j-1}^n - 2C_j^n + C_{j+1}^n}{\Delta x^2} = -C_j^{n+1}, \tag{17}$$

using the same values for the parameters. As can be seen from Figure 1, the proposed method is stable and produces a solution that is very close to the exact solution, but both EE and NSFD methods are unstable for this choice of a time step $\Delta t = 0.005$ and larger. The parameters used in this simulation are taken from [2].



(a) Solutions at $T = 0.85$ (b) Solution of the EE method

(c) Solution of the NSFD method (d) Solution of the new method

Figure 1. *Solutions for the exponential traveling wave model.*

3.2. Example 2: Colonization of Europe by oaks

In the second example, we deal with the model for the recolonization by oaks of Europe after the last glaciation. The model assumes Malthusian growth and a standard advection-diffusion reaction equation for the local density $C(x,t)$ of oaks at time t :

$$\frac{\partial C(x,t)}{\partial t}+u\frac{\partial C(x,t)}{\partial x}-D\frac{\partial^2 C(x,t)}{\partial x^2}=rC(x,t),\qquad (x,t)\in[0,x_{\max}]\times[0,T], \tag{18}$$

where r is the reproduction rate, u is an advection parameter taking into account the displacement of acorns by squirrels, and D is the diffusivity. If the population size at time 0 is M and is concentrated at the origin, the exact solution of this equation is

$$C(x,t)=\frac{M}{2\sqrt{\pi Dt}}\exp\left(rt-\frac{(x-ut)^2}{4Dt}\right), \tag{19}$$

for more details see [2, 5]. In Figure 2 numerical solutions for (18) are shown with $u=1$, $D=1$, $r=0.1$, $x_{\max}=10$, $T=2$, $\Delta x=0.1$ and $\Delta t=0.005$, which are taken from [2]. Comparing the proposed new method with the upwind EE method:

$$\frac{C_j^{n+1}-C_j^n}{\Delta t}+u\frac{C_j^n-C_{j-1}^n}{\Delta x}-D\frac{C_{j-1}^n-2C_j^n+C_{j+1}^n}{\Delta x^2}=rC_j^n, \tag{20}$$

we observe that the new method performs very well. Furthermore, NSFD method for (18), proposed by Mickens in [16], is the same as the EE method.

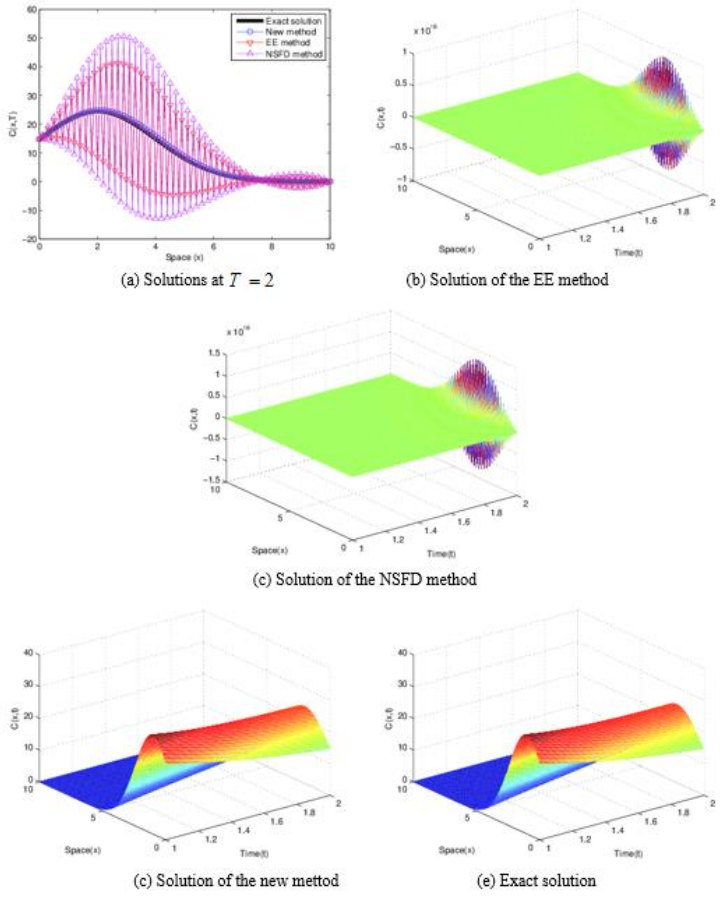


Figure 2. *Solutions for the oak propagation model.*

3.3. Example 3: Catalytic particle

As our third example we consider (1) with $P=Pe$, $Q=1$ and $R=\phi^2$

$$\frac{\partial C(x,t)}{\partial t} + Pe\frac{\partial C(x,t)}{\partial x} - \frac{\partial^2 C(x,t)}{\partial x^2} = -\phi^2 C(x,t), \qquad (x,t) \in [0, x_{\max}] \times [0,T], \tag{21}$$

with initial and boundary conditions

$$C(x,0) = 0, \qquad C(0,\mathrm{t}) = 1, \qquad C(1,\mathrm{t}) = 1. \tag{22}$$

The unknown $C(x,\mathrm{t})$ corresponds to the normalized concentration and endowed, Pe is the *Peclet* number, which denotes the relationship between the advective and diffusive transport and ϕ is Thiele modulus, which relates chemical reaction rate and the diffusive transport; the dimensionless parameters $x \in [0,1]$ and $t > 0$ denote the spatial coordinate and time, respectively.

In traditional FD schemes, the spatial operators of (21) can be discretized in different ways. By *method of lines* (MOL) approach, we replace the spatial derivatives C_x and C_{xx} by a finite difference approximation to arrive at a semi-discrete system where $C_i(\mathrm{t}) \simeq C(x_i,\mathrm{t})$. According to the MOL approach, *fully discrete* approximation $C_i^n \simeq C(x_i,\mathrm{t}_n)$ are now obtained by applying some suitable ordinary differential equations (ODEs) solver. For instance, for an equidistant grid $X_{N+1} = \{x_a, x_1, \cdots, x_N, x_b\}$ where $x_a = 0$ and $x_b = 1$, with $x_i - x_{i-1} = \Delta x$ and For the advective operator, it is also possible to use backward or forward approximations for obtaining the following schemes

- Forward finite difference (FFD) scheme

$$\frac{dC_i(\mathrm{t})}{dt} = \frac{C_{i-1}(\mathrm{t}) - (2 - Pe\Delta x)C_i(\mathrm{t}) + (1 - Pe\Delta x)C_{i+1}(\mathrm{t})}{\Delta x^2} - \phi^2 C_i(\mathrm{t}), \tag{23}$$

- Backward finite difference (BFD) scheme

$$\frac{dC_i(\mathrm{t})}{dt} = \frac{(1 + Pe\Delta x)C_{i-1}(\mathrm{t}) - (2 + Pe\Delta x)C_i(\mathrm{t}) + C_{i+1}(\mathrm{t})}{\Delta x^2} - \phi^2 C_i(\mathrm{t}). \tag{24}$$

To obtain a reference solution of (21) the Laplace transform was applied and for the analytical solution we found

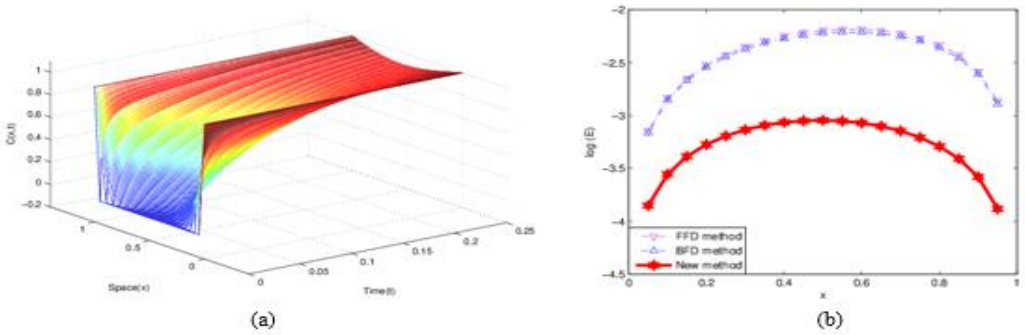
$$\hat{C}(\mathrm{x},\mathrm{s}) = LC(x,t) = \frac{\exp(m_2 x)[\exp(m_1) - 1] + \exp(m_1 x)[1 - \exp(m_2)]}{\exp(m_1) - \exp(m_2)} \tag{25}$$

With

$$m_1 = \frac{Pe - \sqrt{Pe^2 + 4(s + \phi^2)}}{2}, \qquad m_2 = \frac{Pe + \sqrt{Pe^2 + 4(s + \phi^2)}}{2}, \tag{26}$$

where $\hat{C}(x,\mathrm{s})$ is the Laplace transform of $C(x,\mathrm{t})$. Unfortunately, the inverse Laplace transform for $\hat{C}(x,\mathrm{s})$ is not available. In order to determinate the solution in the time-domain, we have used the numerical inversion by Zakians algorithm [23, 24].

We apply new scheme to (21) with $Pe = 1$ and $\phi = 0.1$. Figure 3(a) shows the concentration profile for new scheme. A comparison with the FFD and BFD schemes one can find that new scheme performs well, see Figure 3(b).



(a) (b)

Figure 3. *Solution of the new method (a) and logarithm of absolute errors (b) with* $Pe = 1$ *and* $\phi = 0.1$.

3.4. Example 4: Adsorption of contaminants

Ground water is subject to pollution. Pollutants present on the surface may be carried by water percolating into the ground. The pollutants may come from garbage dumps, septic tanks, industrial or mining waste or even fertilizers, pesticides and herbicides from agricultural or domestic use. Part or all of these pollutants may be adsorbed by the soil before reaching groundwater aquifers. We assume that a nonvolatile trace element is transported by the water phase. Let C be the concentration of the element in the water phase and let q be the concentration in the solid matrix. Following [1], the two balance equations involving C and q , for a nonstationary Langmuir isotherm, are:

$$\begin{cases} \dfrac{\partial C}{\partial t} + u\dfrac{\partial C}{\partial x} - D\dfrac{\partial^2 C}{\partial x^2} = \dfrac{\rho}{\theta}\dfrac{\partial q}{\partial t} \\ \dfrac{\partial q}{\partial t} = k_f C\left(b - q\right) - k_b q \end{cases}, \tag{27}$$

where k_f is the sorption rate constant, b is the maximum solid phase concentration, and k_b is the desorption rate constant, $u = u_\omega / \theta_\omega$ is the pore water velocity, $\rho = \rho_s \theta_s$ is the bulk density of the porous medium, $\theta = \theta_\omega$, θ_ω is the volumetric water content, u_ω is the water-phase velocity, D is the dispersion coefficient, θ_s is the volumetric content of the solid matrix, and ρ_s is the density of the solid matrix. An exact solution for the system (27) given by [7] is the following:

$$C(x,t) = \frac{-\dfrac{a_1}{a_2}}{1 + \exp\left[-a_1\left(x - \alpha u t\right)\right]}, \tag{28}$$

Where

$a_1 = -0.8428$, $a_2 = 0.1876$, $\alpha = 0.1329.$

The values of the parameters, $u = 40.1$, $D = 36.09$, $\rho = 1.64$, $\theta = 0.41$, $k_f = 2.0$, $k_b = 0.643$ and $b = 7.85$, used in our simulation are also taken from [6].

The proposed nonstandard explicit method for system (27) is:

$$\begin{cases} \dfrac{C_j^{n+1}-C_j^n}{\Delta t}+u\dfrac{C_j^n-C_{j-1}^n}{\Delta x}-D\dfrac{C_{j-1}^n-2C_j^n+C_{j+1}^n}{\Delta x^2} \\ \qquad +\dfrac{\rho}{\theta}\left(k_f b\left(a\left(C_{j+1}^n+C_{j-1}^n\right)+(1-2a)C_j^{n+1}\right)-k_f C_j^n q_j^n-k_b q_j^n\right)=0, \\ \dfrac{q_j^{n+1}-q_j^n}{\Delta t}=k_f bC_j^n-k_f C_j^n q_j^{n+1}-k_b q_j^n \end{cases} \tag{29}$$

the system (29) can be written as:

$$\begin{cases} \left(\dfrac{1}{\Delta t}+\dfrac{\rho}{\theta}bk_f(1-2a)\right)C_j^{n+1}=\left(\dfrac{u}{\Delta x}+\dfrac{D}{\Delta x^2}-\dfrac{\rho}{\theta}bk_f a\right)C_{j-1}^n+\left(\dfrac{1}{\Delta t}-\dfrac{u}{\Delta x}-\dfrac{2D}{\Delta x^2}\right)C_j^n \\ \qquad +\left(\dfrac{D}{\Delta x^2}-\dfrac{\rho}{\theta}bk_f a\right)C_{j+1}^n+\dfrac{\rho}{\theta}k_f C_j^n q_j^n+\dfrac{\rho}{\theta}k_b q_j^n \\ \left(\dfrac{1}{\Delta t}+k_f C_j^n\right)q_j^{n+1}=\left(\dfrac{1}{\Delta t}+k_b\right)q_j^n+bk_f C_j^n \end{cases}. \tag{30}$$

The upwind explicit Euler (EE) scheme is:

$$\begin{cases} \dfrac{C_j^{n+1}-C_j^n}{\Delta t}+u\dfrac{C_j^n-C_{j-1}^n}{\Delta x}-D\dfrac{C_{j-1}^n-2C_j^n+C_{j+1}^n}{\Delta x^2}+\dfrac{\rho}{\theta}\left(k_f bC_j^n-k_f C_j^n q_j^n-k_b q_j^n\right)=0 \\ \dfrac{q_j^{n+1}-q_j^n}{\Delta t}=k_f bC_j^n-k_f C_j^n q_j^{n+1}-k_b q_j^n \end{cases}, \tag{31}$$

and the NSFD scheme, proposed by Mickens in [6], is:

$$\begin{cases} \dfrac{C_j^{n+1}-C_j^n}{\Delta t}+u\dfrac{C_j^n-C_{j-1}^n}{\Delta x}-D\dfrac{C_{j-1}^n-2C_j^n+C_{j+1}^n}{\Delta x^2}+\dfrac{\rho}{\theta}\left(k_f bC_j^{n+1}-k_f C_j^n q_j^n-k_b q_j^n\right)=0 \\ \dfrac{q_j^{n+1}-q_j^n}{\Delta t}=k_f bC_j^{n+1}-k_f C_j^{n+1}q_j^{n+1}-k_b q_j^{n+1} \end{cases}. \tag{32}$$

The values used for these calculations are $\Delta x=0.1$, $\Delta t=0.0002$, the model was solved in $(x,t)\in[-20,60]\times[0,T]$ and $T=0.008$. In Figure 4 numerical approximations of the (27) have been shown with the proposed scheme. The new scheme is stable and positive at time T, while the approximations obtained by the EE (31) and NSFD (32) methods are unstable.

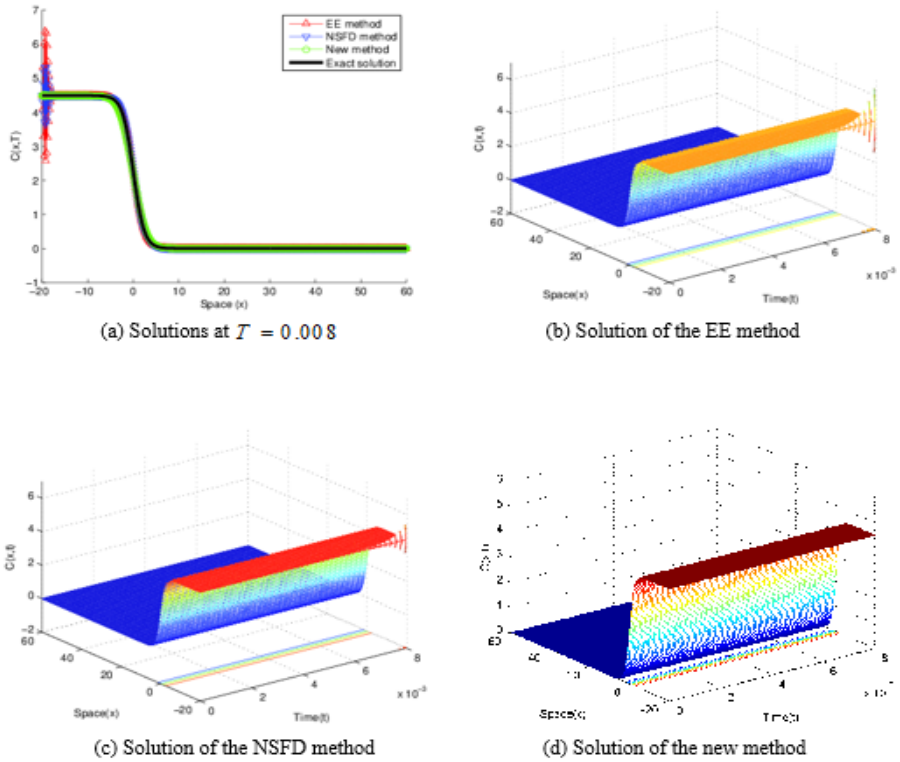


Figure 4. *Solutions for the adsorption model.*

4. CONCLUSIONS AND DISCUSSION

Schemes preserving the positivity are great importance. Such schemes can be employed to prevent the occurrence of negative values where even very small negative values are unacceptable. Within the strategy suggested by Mickens, consisting of a combined use of different finite difference schemes in order to satisfy all the severe requirements of the problem, we have presented a family of NSFD scheme that is positivity preserving. We have presented thenew method for an advection-diffusion reaction equation with constant velocity and diffusion and different reactions in one spatial dimension. Comparisons with a standard explicit upwind Euler (EE) method and with the Mickens′ NSFD method, show that our NSFD method performs very well and it is stable under conditions for which the other methods are very unstable. We studied the suffusion conditions on positivity for the new method. A future work can be investigate the necessity of condition for positivity in Theorem 1.

CONFLICT OF INTEREST

No conflict of interest was declared by the authors

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