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Positivity-preserving nonstandard finite difference schemes for simulation of advection-diffusion reaction equations

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Abstract Systems in which reaction terms are coupled to diffusion and advection transports arise in a wide range of chemical engineering applications, physics, biology and environmental. In these cases, the components of the unknown can denote concentrations or population sizes which represent quantities and they need to remain positive. Classical finite difference schemes may produce numerical drawbacks such as spurious oscillations and negative solutions because of truncation errors and may then become unstable. We propose a new scheme that guarantees a smooth numerical solution, free of spurious oscillations and satisfies the positivity requirement, as is demanded for the advection-diffusion reaction equations. The method is applicable to both advection and diffusion dominated problems. We give some examples from different applications.

Keywords. Nonstandard finite differences, Positivity, Advection-diffusion reaction equation, M-matrix.

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1. Introduction

When one solves differential equations, modeling physical or biological phenomena, it is of great importance to take physical constraints into account. More precisely, numerical schemes have to be designed such that discrete solutions satisfy the same constraints as exact solutions such as positivity, monotonicity and total variation dimensioning, see for examples [3, 6, 7, 10, 11, 20]. Numerical schemes are not usually constructed to satisfy those properties explicitly.

Parabolic equations with or without reaction terms are used extensively in the modeling of many physical and biological phenomena such as heat transfer, transport

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and reaction of chemical species and population density in mathematical biology. They constitute a central component in applied mathematics and their numerical simulations are fundamental importance in gaining the correct qualitative and quantitative information on the systems. Since the quantities that are being modeled, concentrations of chemical species and populations sizes are necessarily positive, it is important to have numerical schemes that preserve the positivity of the solution. Numerical methods based on standard finite difference (SFD) or finite element discretizations are widely used, see for example [3,21]. They do not explicitly incorporate the requirement that the solutions be positive. Even though these schemes guarantee convergence of the discrete solution to the exact one, but some times occurs that the essential qualitative properties such as positivity and monotonicity of the solutions are not transferred to the numerical solution. One way of avoiding this disadvantage is to imply finite difference schemes that are nonstandard in the sense of Mickens' definition [13].

Nonstandard finite differences methods (NSFDs) in addition to the usual properties of consistency, stability and hence convergence, produce numerical solutions which also exhibit essential properties of solutions [2,8,9,12,14–17]. In this paper we propose a new class of NSFD schemes for advection-diffusion-reaction equations by using nonlocal approximation of reaction term. The proposed scheme enable us to solve accurately the examined problems. An important factor for new method is the *positivity preservation* of the solution which exhibit essential property of solutions.

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 three problems and compared with SFD schemes. Finally we end the paper with some conclusions in Section 4.

2. Scheme construction

The relevant partial differential equation in this study is given as follows

$$\frac{\partial C(x,t)}{\partial t} + P\frac{\partial C(x,t)}{\partial x} - Q\frac{\partial^2 C(x,t)}{\partial x^2} = -RC(x,t), \quad (x,t) \in [0, x_{max}] \times [0,T], \tag{2.1}$$

for the unknown $C = C(x,t)$, with appropriate boundary and initial conditions and where the parameters P, Q and R are positive constants.

Take a partition of the interval $[0, x_{max}]$, $x_0 < x_1 < \cdots < x_N$ with $x_j = j\Delta x$, $j = 0, 1, \cdots, N$ and $\Delta x = x_{max}/N$ and divide the time interval of interest $[0,T]$ using equal time steps of size $\Delta t = T/M$ with $t_n = n\Delta t$, $n = 0, 1, \cdots, M$. Let C_j^n be the

approximation to $C(x_j, t_n)$. Here j and n are positive integers.
Making use of the nonstandard discretization of the reaction term $RC(x,t)$ in (2.1), it is now desired to find an accurate NSFD scheme which is positivity preserving and can be written as

$$C(x,t) = a(C_{j+1}^{n+1} + C_{j-1}^{n+1}) + (\frac{1}{2} - a)(C_{j+1}^{n} + C_{j-1}^{n}), \tag{2.2}$$

where a is arbitrary parameter to be determined below. The corresponding finite difference approximation provides the equation difference

$$PC^{n+1} = NC^n, \tag{2.3}$$

where P and N are the following tridiagonal matrices

$$P = tridiag\left\{-\frac{P}{2\Delta x} - \frac{Q}{\Delta x^2} + aR; \frac{1}{\Delta t} + \frac{2Q}{\Delta x^2}; \frac{P}{2\Delta x} - \frac{Q}{\Delta x^2} + aR\right\}, \tag{2.4}$$

$$N = tridiag\left\{-(\frac{1}{2} - a)R; \frac{1}{\Delta t}; -(\frac{1}{2} - a)R\right\}. \tag{2.5}$$

The parameter a is chosen according to the following theorem.

Theorem 1. If $\frac{1}{2} \leq a \leq \frac{\frac{Q}{\Delta x^2} - \frac{P}{2\Delta x}}{R}$, then the scheme (2.3) is unconditionally positive.

Proof. From (2.3) it is enough to show that $P^{-1} > 0$ and $N \geq 0$.

- Since, P is an M-matrix, see [23], then we have to put

$$-\frac{P}{2\Delta x} - \frac{Q}{\Delta x^2} + aR \leq 0, \tag{2.6}$$

$$\frac{P}{2\Delta x} - \frac{Q}{\Delta x^2} + aR \leq 0, \tag{2.7}$$

and $P^{-1} > 0$, see [1].
From (2.6) we can write

$$a \leq \frac{\frac{Q}{\Delta x^2} + \frac{P}{2\Delta x}}{R}, \tag{2.8}$$

and From (2.7) we can write

$$a \leq \frac{\frac{Q}{\Delta x^2} - \frac{P}{2\Delta x}}{R}. \tag{2.9}$$

- In order to nonnegativity for N, we write

$$-(\frac{1}{2} - a)R \geq 0 \quad \text{then} \quad a \geq \frac{1}{2}. \tag{2.10}$$

Then, from (2.8), (2.9) and (2.10) we have

$$\frac{1}{2} \leq a \leq \frac{\frac{Q}{\Delta x^2} - \frac{P}{2\Delta x}}{R}, \tag{2.11}$$

and this completes the proof. □

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

Proof. Under condition (2.11), $P = [p_{ij}]$ is similar to a symmetric tridiagonal matrix (see e.g. [22, p. 24]), so that the eigenvalues of P, $\lambda_i(P), i = 1, \cdots, N$ are real. Also P is row diagonally dominant with $\delta_i = |p_{ii}| - \sum_{j \neq i} |p_{ij}| = \frac{1}{\Delta t} + 2Ra > 0$. So $\|P^{-1}\|_\infty \leq \frac{1}{\frac{1}{\Delta t} + 2Ra}$ (see e.g. [22, p. 8]) and by combining with $\|N\|_\infty = \frac{1}{\Delta t} + 2Ra - R$, we have

$$\rho(P^{-1}N) \leq \|P^{-1}N\|_\infty \leq \|P^{-1}\|_\infty \|N\|_\infty \leq \frac{\frac{1}{\Delta t} + 2Ra - R}{\frac{1}{\Delta t} + 2Ra} < 1. \tag{2.12}$$

where $\rho(P^{-1}N)$ is the spectral radius of the matrix $P^{-1}N$. Therefor the scheme is stable and then via the Lax-theorem convergent with local truncation error

$$\begin{aligned} T_j^n =& \frac{C_j^{n+1} - C_j^n}{\Delta t} + P\frac{C_{j+1}^{n+1} - C_{j-1}^{n+1}}{2\Delta x} - Q\frac{C_{j-1}^{n+1} - 2C_j^{n+1} + C_{j+1}^{n+1}}{\Delta x^2} \\ &+ R\Big(a(C_{j+1}^{n+1} + C_{j-1}^{n+1}) + (\frac{1}{2} - a)(C_{j+1}^n + C_{j-1}^n)\Big), \end{aligned} \tag{2.13}$$

by Taylor's expansion

$$\begin{aligned} C_j^{n+1} &= C_j^n + \Delta t\frac{\partial C_j^n}{\partial t} + \frac{1}{2}\Delta t^2\frac{\partial^2 C_j^n}{\partial t^2} + \frac{1}{6}\Delta t^3\frac{\partial^3 C_j^n}{\partial t^3} + \cdots, \\ C_{j+1}^n &= C_j^n + \Delta x\frac{\partial C_j^n}{\partial x} + \frac{1}{2}\Delta x^2\frac{\partial^2 C_j^n}{\partial x^2} + \frac{1}{6}\Delta x^3\frac{\partial^3 C_j^n}{\partial x^3} + \cdots, \\ C_{j-1}^n &= C_j^n - \Delta x\frac{\partial C_j^n}{\partial x} + \frac{1}{2}\Delta x^2\frac{\partial^2 C_j^n}{\partial x^2} - \frac{1}{6}\Delta x^3\frac{\partial^3 C_j^n}{\partial x^3} + \cdots, \\ C_{j+1}^{n+1} &= C_j^n + \Delta x\frac{\partial C_j^n}{\partial x} + \Delta t\frac{\partial C_j^n}{\partial t} + \frac{1}{2}\Delta x^2\frac{\partial^2 C_j^n}{\partial x^2} + \frac{1}{2}\Delta t^2\frac{\partial^2 C_j^n}{\partial t^2} + \Delta x\Delta t\frac{\partial^2 C_j^n}{\partial x \partial t} + \cdots, \\ C_{j-1}^{n+1} &= C_j^n - \Delta x\frac{\partial C_j^n}{\partial x} + \Delta t\frac{\partial C_j^n}{\partial t} + \frac{1}{2}\Delta x^2\frac{\partial^2 C_j^n}{\partial x^2} + \frac{1}{2}\Delta t^2\frac{\partial^2 C_j^n}{\partial t^2} - \Delta x\Delta t\frac{\partial^2 C_j^n}{\partial x \partial t} + \cdots, \end{aligned}$$

and by substitution into (2.13) we have

$$T_j^n = \left(\frac{\partial C}{\partial t} + Pe\frac{\partial C}{\partial x} - \frac{\partial^2 C}{\partial x^2} + RC\right)_j^n + \frac{1}{2}\Delta t\frac{\partial^2 C_j^n}{\partial t^2} + \frac{1}{2}R(a+\frac{1}{2})\Delta x^2\frac{\partial^2 C_j^n}{\partial x^2} + \cdots, \tag{2.14}$$

hence the difference is consistent with (2.1) and $T_j^n = O(\Delta t + \Delta x^2)$. These conclude the theorem.□

3. Test cases

In this section we perform numerical experiments to demonstrate the performance of the new proposed scheme with respect to positivity and stability, developed in the previous section. Several test cases were run to assess the performance of this positivity-preserving NSFD scheme. We validate the method by comparing its results with exact solutions and also with solutions obtained by other methods.

3.1. **Test case 1: Catalytic particle.** First we have considered (2.1) with $Q = 1$, $R = \phi^2$ and two different values for P:

$$\frac{\partial C(x,t)}{\partial t} + P\frac{\partial C(x,t)}{\partial x} - \frac{\partial^2 C(x,t)}{\partial x^2} = -\phi^2 C(x,t), \quad (x,t) \in [0, x_{max}] \times [0,T], \tag{3.1}$$

with initial and boundary conditions

$$C(x,0) = 0, \quad C(0,t) = 1, \quad C(1,t) = 1. \tag{3.2}$$

The unknown $C(x,t)$ corresponds to the normalized concentration and endowed, P 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 (3.1) 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 $C_i(t) \simeq C(x_i,t)$. According to the MOL approach, *fully discrete* approximation $C_i^n \simeq C(x_i,t_n)$ 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

$$\frac{dC_i(t)}{dt} = \frac{C_{i-1}(t) - (2 - P\Delta x)C_i(t) + (1 - P\Delta x)C_{i+1}(t)}{\Delta x^2} - \phi^2 C_i(t). \tag{3.3}$$

- Backward finite difference (BFD) scheme

$$\frac{dC_i(t)}{dt} = \frac{(1 + P\Delta x)C_{i-1}(t) - (2 + P\Delta x)C_i(t) + C_{i+1}(t)}{\Delta x^2} - \phi^2 C_i(t). \tag{3.4}$$

To obtain a reference solution of (3.1) the Laplace transform was applied and for the analytical solution we found

$$\hat{C}(x,s) = LC(x,t) = \frac{\exp(m_2 x)[\exp(m_1) - 1] + \exp(m_1 x)[1 - \exp(m_2)]}{\exp(m_1) - \exp(m_2)} \tag{3.5}$$

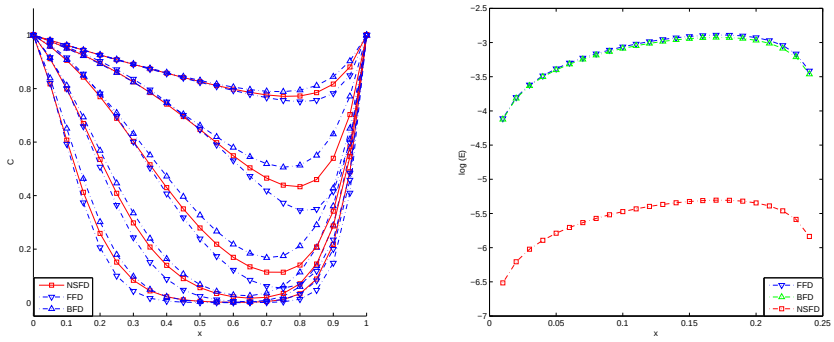
with

$$m_1 = \frac{P - \sqrt{P^2 + 4(s + \phi^2)}}{2} \quad , \quad m_2 = \frac{P + \sqrt{P^2 + 4(s + \phi^2)}}{2}, \tag{3.6}$$

where $\hat{C}(x,s)$ is the Laplace transform of $C(x,t)$. Unfortunately, the inverse Laplace transform for $\hat{C}(x,s)$ is not available. In order to determinate the solution in the time-domain, we have used the numerical inversion by Zakians algorithm [22, 24].
We apply new scheme to (3.1) with different values of P and ϕ. Several studies indicated that numerical results of standard finite difference methods lead to numerical dispersions in the advection dominated problems [5, 18, 19, 25]. Figure 1 shows the concentration profiles and their respective errors. As a expected for a wide range of P and ϕ, classical FD schemes provide a bigger approximation errors than the new NSFD scheme and for small values of P (≤ 1) and ϕ, better agreements between the FD schemes and new scheme are observed, see Figure 2(a). However, in this case new scheme performs well, see Figure 2(b).

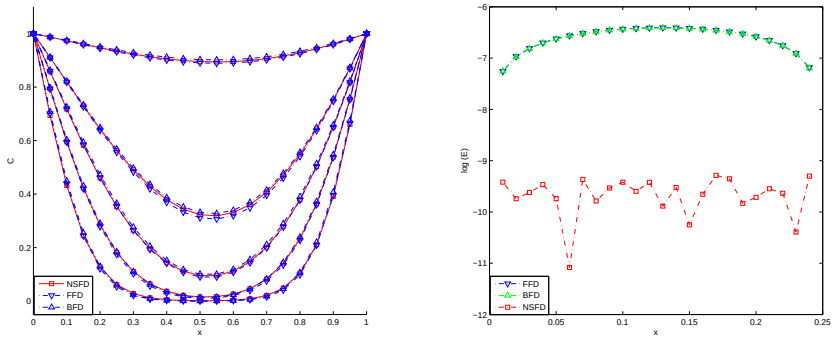
3.2. **Test case 2: Exponential traveling wave.** The second test case consists of equation (2.1) for $P = 1$, $Q = 1$ and $R = 1$:

$$\frac{\partial C(x,t)}{\partial t} + \frac{\partial C(x,t)}{\partial x} - \frac{\partial^2 C(x,t)}{\partial x^2} = -C(x,t), \quad (x,t) \in [0, x_{max}] \times [0, T], \tag{3.7}$$



(a) (b)

FIGURE 1. Concentration profiles at different times and logarithm of absolute errors with $P = 10$ and $\phi = 2$.



(a) (b)

FIGURE 2. Concentration profiles at different times and logarithm of absolute errors with $P = 1$ and $\phi = 0.1$.

with initial condition

$$C(x, 0) = \exp(-x), \quad x \in [0, x_{max}], \tag{3.8}$$

and boundary conditions

$$C(0,t) = \exp(t), \quad t \in [0,T],$$
$$\frac{\partial C(x_{max},t)}{\partial x} = -C(x_{max},t), \quad t \in [0,T]. \tag{3.9}$$

The exact solution is given by

$$C(x,t) = \exp(t-x). \tag{3.10}$$

In order to show the advantages of the proposed new method, we numerically solve (3.7) 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)

$$\frac{C_j^{n+1} - C_j^n}{\Delta t} + \frac{C_j^n - C_{j-1}^n}{\Delta x} - \frac{C_{j-1}^n - 2C_j^n + C_{j+1}^n}{\Delta x^2} = -C_j^n, \tag{3.11}$$

and by the nonstandard finite-difference (NSFD) method, proposed by Mickens in [14]

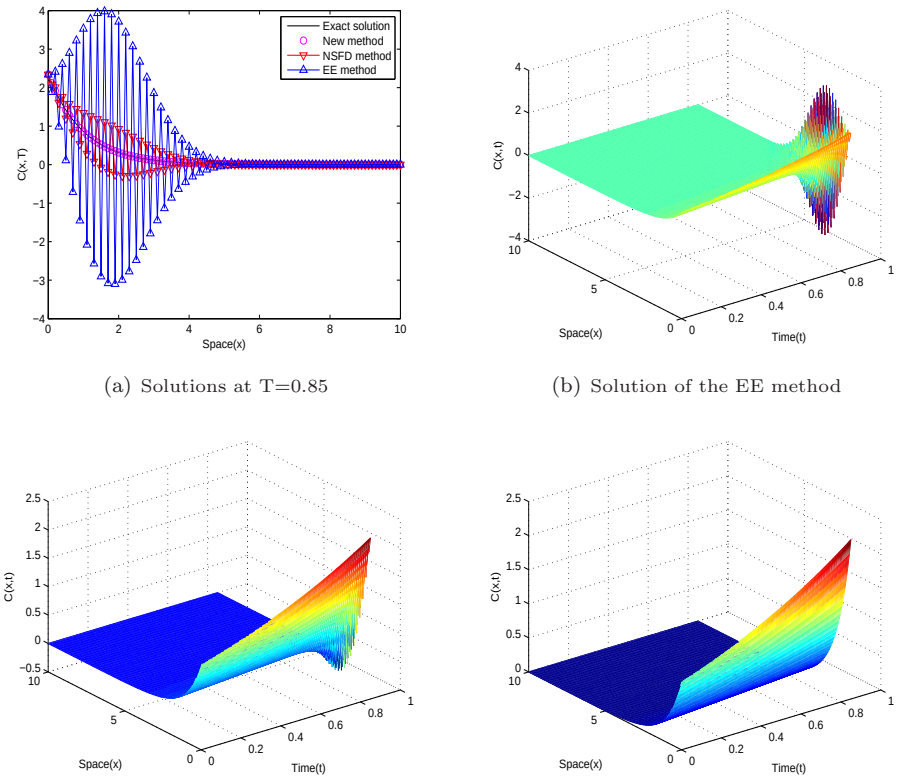
$$\frac{C_j^{n+1} - C_j^n}{\Delta t} + \frac{C_j^n - C_{j-1}^n}{\Delta x} - \frac{C_{j-1}^n - 2C_j^n + C_{j+1}^n}{\Delta x^2} = -C_j^{n+1}, \tag{3.12}$$

using the same values for the parameters. As can be seen from Figure 3, 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.

3.3. **Test case 3: Colonization of Europe by oaks.** In the third test case, 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

$$\frac{\partial C(x,t)}{\partial t} + u\frac{\partial C(x,t)}{\partial x} - D\frac{\partial^2 C(x,t)}{\partial x^2} = rC(x,t), \quad (x,t) \in [0,x_{max}] \times [0,T], \tag{3.13}$$

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



(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 3. Solutions for the exponential traveling wave model.

time 0 is M and is concentrated at the origin, the exact solution of this equation is

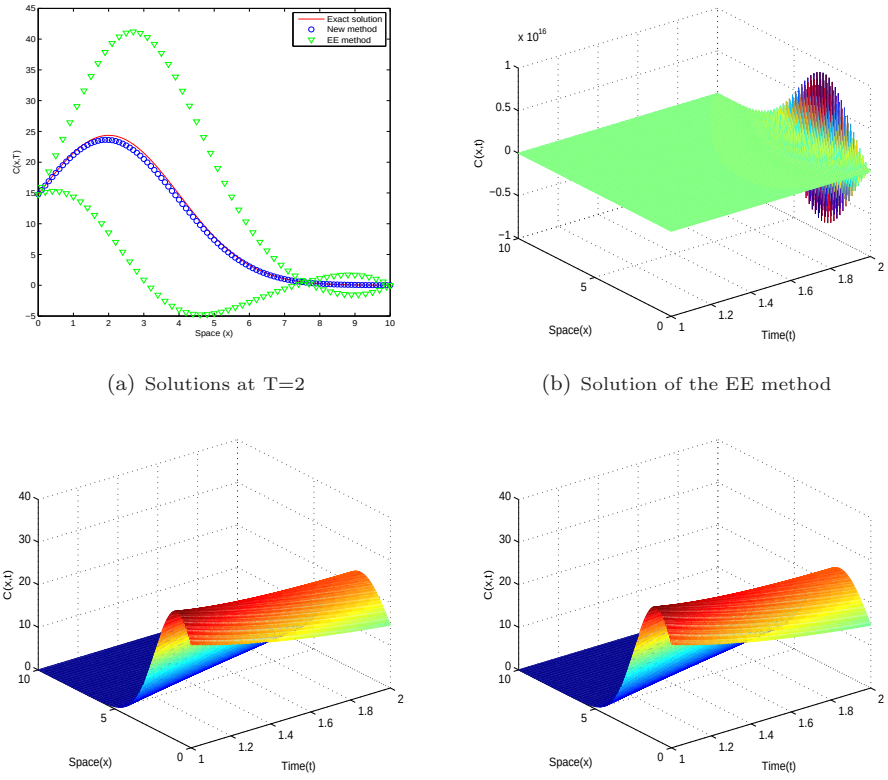
$$C(x,t) = \frac{M}{2\sqrt{\pi D t}} \exp\left(rt - \frac{(x-ut)^2}{4Dt}\right), \tag{3.14}$$

for more details see [4].

In Figure 4 numerical solutions for (3.13) are shown with $u = 1$, $D = 1$, $r = 0.1$, $x_{max} = 10$, $T = 2$, $\Delta x = 0.1$ and $\Delta t = 0.005$. Comparing the proposed new method with the upwind EE method

$$\frac{C_j^{n+1} - C_j^n}{\Delta t} + u\frac{C_j^n - C_{j-1}^n}{\Delta x} - D\frac{C_{j-1}^n - 2C_j^n + C_{j+1}^n}{\Delta x^2} = rC_j^n, \tag{3.15}$$

we observe that the new method performs very well. Furthermore, NSFD method for (3.13), proposed by Mickens in [14], is the same as the EE method.



(a) Solutions at T=2

(b) Solution of the EE method

(c) Solution of the new method

(d) Exact solution

FIGURE 4. Solutions for the oak propagation 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 strategy of nonlocal approximation, we have presented a NSFD scheme. The proposed scheme has local truncation error $O(\Delta t, \Delta x^2)$, but works successfully, and it is positivity preserving. We have presented the new 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 a nonstandard finite-difference 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 sufficient conditions

on positivity for the new method. A future work can be investigate the necessity of condition for positivity in Theorem 1.

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