

Non-Standard Finite Difference Schemes for Michaelis-Menten type Reaction Diffusion Equations

Michael Chapwanya¹, Jean M-S Lubuma^{1*} and Ronald E Mickens²

¹Department of Mathematics and Applied Mathematics, University of Pretoria
Pretoria 0002, South Africa, (m.chapwanya@up.ac.za, jean.lubuma@up.ac.za)

²Department of Physics, Clark Atlanta University
Atlanta GA 30314, USA, (rohrrs@math.gatech.edu)

Abstract

We compare and investigate the performance of the exact scheme of the Michaelis-Menten (M-M) ordinary differential equation with several new non-standard finite difference (NSFD) schemes that we construct by using Mickens' rules. Furthermore, the exact scheme of the M-M equation is used to design several dynamically consistent NSFD schemes for related reaction-diffusion equations, advection-reaction equations and advection-reaction-diffusion equations. Numerical simulations that support the theory and demonstrate computationally the power of NSFD schemes are presented.

AMS Subject Classification (2010): 65L12; 65L99; 65M06; 65M99

Keywords: nonstandard finite difference method, exact scheme, Lambert W function, Michaelis-Menten equation, advection-reaction-diffusion equations

1 Introduction

The Michaelis-Menten (M-M) ordinary differential equation

$$\frac{du}{dt} = -\frac{u}{1+u},$$

is of great interest in applications. It models the enzyme kinetics in pharmacology and was solved in [1] and [2] with a singular perturbation technique where u is one of the leading order terms of the expansion of the outer solution. The right-hand side of the M-M equation also arises in predator-prey and infectious disease models as a functional response in specific extended forms ranging from the Michaelis-Menten-type, the ratio-dependent-type, the Beddington-De Angelis-type, to the general Holling type II considered in the Rosenzweig-Mac Arthur model (see, for instance, [3] and [4]).

The M-M equation is simple in mathematical structure. However, its solutions cannot be found explicitly. Thus, there has been a surge in the construction of numerical methods that can provide useful and reliable information on this differential model. The particular type of information and properties on which many researchers have focused are the linear stability of the the hyperbolic critical point $\tilde{u} = 0$ and the positivity of the solutions. Nonstandard Finite Difference (NSFD) schemes, which are elementary stable and preserve the positivity of the exact solutions have been extensively investigated for general dynamical systems including the M-M equation and the combustion model (see the books [5], [6] and [7] and the references therein).

The point of departure of the current work is the exact scheme of the M-M equation, which was designed only recently by Mickens [8]. The exact scheme is based on a general existence theorem in [5, p. 71] that is applicable in this case, thanks to the so-called Lambert W function which permits us to write the solution of the M-M equation in a compact form [9]. Furthermore, given the specific nature of the M-M functional response, we construct three new NSFD schemes, which are

*Corresponding author: jean.lubuma@up.ac.za

all topologically dynamically consistent in the sense of [10]. The analysis is taken one step further by designing various NSFD schemes for the major related reaction-partial differential equations of which the M-M model is the limit equation in the space independent case. This is done by using Mickens' rules [5]. One focus of the work is to provide the details of the numerical solutions for the M-M equation by comparing and investigating the performance of the exact scheme, the exact scheme-related methods and other NSFD schemes. The focus on detailed theoretical and computational proofs distinguishes our work from previous work in the literature, where the emphasis is just on plugging the M-M equation into one of the standard ODE solvers. In this regard, we can mention the relatively recent work [11] (and the references therein), where numerically integrated solutions of the M-M equation are considered, without details.

The rest of the paper is organized as follows. In the next section, we recall the definition of the Lambert W function, the main tool we use in this work. The M-M equation is discussed at length in Sect. 3 where we study its exact scheme and compare the performance with three new NSFD schemes. NSFD schemes for the M-M conservative oscillator or Hamiltonian system are investigated in Sect. 4. Sects. 5, 6 and 7 are devoted to the analysis of NSFD schemes for the M-M reaction-diffusion equation, the M-M advection-reaction equation and the M-M advection-reaction-diffusion equation, respectively. Numerical simulations that illustrate the power of all our NSFD schemes are presented in Sect. 8. Sect 9 provides concluding remarks pertaining to how the new NSFD schemes fit in the literature and how the study can be extended.

2 The Lambert W Function

Special functions play such an important role in science and engineering that there are many handbooks on them in the literature and most of these are user friendly (e.g. [12, 13]). In this work, we will extensively use the Lambert W function, also called the Omega function or the product log, given by the relation

$$z = W(z) \exp(W(z)), \quad (1)$$

as the multivalued inverse of the non-injective complex-valued function

$$w \mapsto w \exp(w).$$

The canonical reference for the Lambert W function is [9] where it is comprehensively studied. In the numerical simulations, we will use the Matlab built-in function "lambertw(*)". Since we will be dealing with the dynamics of systems that are defined on \mathbb{R}_+ , we restrict ourselves to nonnegative real arguments $z \geq 0$ and thus are interested in the (principal) branch satisfying $W(z) \geq 0$, which is a single-valued function.

Often special functions are characterized by differential equations. In the case under consideration, implicit differentiation of (1) shows that W satisfies the differential equation

$$\frac{dW}{dz} = \frac{W(z)}{z(1+W(z))}. \quad (2)$$

3 The Michaelis-Menten ODE

The Michaelis-Menten (M-M) ordinary differential equation (ODE) is

$$\frac{du}{dt} = -\frac{au}{1+bu}, \quad a > 0, \quad b \geq 0, \quad (3)$$

with initial condition

$$u(0) = u^0. \quad (4)$$

Equation (3) arises in pharmacology models of the basic enzyme reaction. The theory of enzyme kinetics and of the M-M equation, which comes from a singularly perturbed system of ODE's, can be found in [14]. The decay equation

$$\frac{du}{dt} = -au, \quad a > 0, \quad (5)$$

is the linearized form of (3) about its unique fixed-point $\tilde{u} = 0$. In what follows, it is more instructive to look at (5) as the comparison equation associated with (3) (see [15]). Considered with the same initial condition in (4), the equations (5) and (3) have exact solutions

$$\underline{u}(t) = \exp(-at)u^0, \quad (6)$$

and

$$u(t) = \frac{1}{b}W((b \exp(-at)u^0 \exp(bu^0))), \quad (7)$$

respectively. The closed form expression (7), based of the Lambert W function, for the solution of the M-M equation is established in [9]. From these exact solutions, we deduce the following intrinsic properties of the M-M model:

Theorem 1 *For a given initial value $u^0 \geq 0$, we have*

$$0 \leq \underline{u}(t) \leq u(t) \leq u^0, \forall t \geq 0, \quad (8)$$

$$\lim_{b \rightarrow 0} u(t) = \underline{u}(t), \forall t \geq 0, \quad (9)$$

and

$$u(t) \downarrow 0 \text{ as } t \rightarrow \infty, \quad (10)$$

where the latter notation means that the function $u(t)$ decreases monotonically to the hyperbolic fixed-point 0 as $t \rightarrow +\infty$.

Remark 2 *In view of the sign of the right hand side of Eq. (3), the hyperbolic fixed point $\tilde{u} = 0$ is locally asymptotically stable. However, Theorem 1 says more than this local property. In particular the differential equation (3) defines a dynamical system on the positive interval $[0, \infty)$, with the fixed-point $\tilde{u} = 0$ being globally asymptotically stable.*

The property (9) is obtained by using (1) where $\lim_{z \rightarrow 0} \frac{W(z)}{z} = 1$. Notice that the relation $\underline{u}(t) \leq u(t)$ in (8) is an illustration of a well-known monotonicity result (see Theorem 8.XI in [16]). Thus for $0 < u^0 < \infty$, all trajectories are bounded and decrease monotonically to zero and $\underline{u} \equiv 0$ is locally asymptotically stable fixed-point.

Let us consider a sequence $\{t_k = k\Delta t\}_{k \geq 0}$ of equally-spaced time points where the parameter $\Delta t > 0$ is the step size. We denote by u^k an approximation to the solution u at the point $t = t_k$.

The design of an exact scheme for the M-M model has been considered only recently, namely in Mickens [8]. Setting from (7), $u^k = u(t_k)$, Mickens proposed for the M-M model, along the lines of [5], the exact scheme that reads as follows:

$$u^{k+1} = \frac{1}{b}W((b \exp(-a\Delta t)u^k \exp(bu^k))). \quad (11)$$

In order to write (11) as a non-standard finite difference (NSFD) scheme, we observe that the exact scheme

$$\underline{u}^{k+1} = \exp(-a\Delta t)\underline{u}^k, \quad (12)$$

for the decay equation is equivalent to

$$\frac{\underline{u}^{k+1} - \underline{u}^k}{\phi_1(\Delta t)} = -a\underline{u}^{k+1}, \quad (13)$$

or

$$\frac{u^{k+1} - u^k}{\phi_2(\Delta t)} = -au^k, \quad (14)$$

where

$$\phi_1(\Delta t) = \frac{\exp(a\Delta t) - 1}{a} \text{ and } \phi_2(\Delta t) = \frac{1 - \exp(-a\Delta t)}{a}. \quad (15)$$

In view of the property (9), that must be replicated by the numerical methods, the equivalent form

$$\frac{u^{k+1} - u^k}{\phi_2(\Delta t)} = \frac{W((b \exp(-a\Delta t)u^k \exp(bu^k)) - bu^k}{b\phi_2(\Delta t)}, \quad (16)$$

which is indeed a NSFD method, is obtained for the exact scheme (11) (see [8]). With the formulation (16), it is readily seen from the mean-value theorem and (2) that

$$\begin{aligned} \frac{W((b \exp(-a\Delta t)u^k \exp(bu^k)) - bu^k)}{b\phi_2(\Delta t)} &= \frac{W((b \exp(-a\Delta t)u^k \exp(bu^k)) - W(bu^k \exp(bu^k)))}{b\phi_2(\Delta t)} \\ &\approx \frac{-au(t_k)}{1 + bu(t_k)}. \end{aligned}$$

Exact schemes that are effective in applications do not exist in many cases. Therefore, using Mickens' rules [5], we also consider the following NSFD schemes for the M-M equation:

$$\frac{u^{k+1} - u^k}{\phi_1(\Delta t)} = -\frac{au^{k+1}}{1 + bu^k}; \quad (17)$$

$$\frac{u^{k+1} - u^k}{\phi_1(\Delta t)} = -\frac{au^{k+1}}{1 + bu^{k+1}}; \quad (18)$$

$$\frac{u^{k+1} - u^k}{\phi_2(\Delta t)} = -\frac{au^k}{1 + bu^k}. \quad (19)$$

By analogy with the continuous model, we denote the sequence (u^k) in (17)–(19) by (\underline{u}^k) when $b = 0$. Thus, each \underline{u}^k is a discrete solution of the decay equation (5). Despite its apparent implicit structure, the NSFD scheme (18), where we are interested in positive discrete solutions, admits the equivalent explicit form in (21) below.

Our aim is to investigate and compare the performance of the NSFD schemes (17), (18) and (19) with the exact scheme (16). In particular, we are interested in determining if the properties in Theorem 1 hold.

Theorem 3 *The NSFD schemes (17)–(19) are dynamically consistent with all the properties stated in Theorem 1. More precisely, for $u^0 \geq 0$ and any $\Delta t > 0$, we have*

$$0 \leq \underline{u}^k \leq u^k \leq u^0, \forall k \geq 0,$$

$$\lim_{b \rightarrow 0} u^k = \underline{u}^k, \forall k \geq 0$$

and

$$u^k \downarrow 0 \text{ as } k \rightarrow \infty.$$

Proof. We prove the theorem for the NSFD scheme (18), the situation being much easier for the other two schemes (17) and (19). Equation (18), with the explicit expression of the denominator function in (15), is quadratic in u^{k+1} in the sense that

$$b(u^{k+1})^2 + (e^{a\Delta t} - bu^k)u^{k+1} - u^k = 0. \quad (20)$$

We assume that $u^k > 0$. Then, the algebraic equation (20) has a negative and a positive roots. The required positive root or solution of (18) is

$$u^{k+1} = \begin{cases} \frac{bu^k - e^{a\Delta t} + \sqrt{(bu^k - e^{a\Delta t})^2 + 4bu^k}}{2b} & \text{if } b > 0 \\ u^k e^{a\Delta t} & \text{if } b = 0. \end{cases} \quad (21)$$

From (18) and the definition of ϕ_1 in (15), we have

$$e^{-a\Delta t}u^k \leq u^{k+1} = \frac{u^k}{1 + (e^{a\Delta t} - 1)(1 + bu^{k+1})^{-1}} \leq u^k, \quad (22)$$

which, for $k = 0$, yields

$$0 \leq \underline{u}^1 = e^{-a\Delta t}u^0 \leq u^1 \leq u^0.$$

Proceeding by mathematical induction on k , we obtain the first claim in the theorem. The other two claims follow from (21) and the decreasing property of the sequence (u^k) in (22). ■

Remark 4 For most of the schemes studied below, we will primarily be interested in the preservation of the positivity of solutions, which is the more relevant property from the practical point of view. However, similarly to Remark 2 for the continuous case, Theorem 3 states much more than the local property of elementary stability of all the NSFD schemes (17)–(19), which simply means that these schemes have $\tilde{u} = 0$ only as a fixed-point and this fixed-point is locally asymptotically stable as for the continuous model (see, e.g. [17] and [5]). In particular, $\tilde{u} = 0$ is globally asymptotically stable. Furthermore, since each one of the NSFD schemes (17)–(19) can be written in the form $u^{k+1} = G(\Delta t; u^k)$ where in each case the function G satisfies the conditions

$$G(0; u) = u \text{ and } \frac{dG(\Delta t; u)}{du} > 0,$$

we have in fact for any value of Δt the replication of all topological dynamical properties, a concept introduced in [10], where it is referred to as topological dynamic consistency. On the contrary, the standard finite difference scheme

$$\frac{u^{k+1} - u^k}{\Delta t} = -\frac{au^k}{1 + bu^k}, \quad (23)$$

is known to be elementary unstable (see, e.g., [5]). It is clear that this standard scheme fails to have positive solutions and to satisfy all the above properties for arbitrary values of Δt . On the other hand, the NSFD schemes (17)–(19) are not constructed in a random way. For instance, if instead of (17), we consider the NSFD scheme

$$\frac{u^{k+1} - u^k}{\phi_1(\Delta t)} = -\frac{au^k}{1 + bu^{k+1}},$$

then, on writing it in the equivalent form similar to (20), it is easy to check that there exists no positive solution u^{k+1} when $u^k > 0$.

Remark 5 While there is actually no need for all three NSFD schemes, each is, however, a valid scheme in its own and of themselves. Nevertheless, we opted to display the three schemes for the purposes of completeness, specifically that concerns on systematic methodologies of constructing NSFD schemes are often raised in the literature. Among other things, the schemes show the natural way of constructing the denominator functions $\phi_i(\Delta t)$.

4 The M-M Hamiltonian system

The steady-state of the reaction diffusion equations to be considered in this work is governed by the second-order differential equation

$$\frac{d^2u}{dx^2} - \frac{au}{1 + bu} = 0, \quad a > 0, \quad b \geq 0, \quad (24)$$

which involves the Michaelis-Menten reaction term. The trivial steady-state $\tilde{u} = 0$ is found to be unstable, since the hyperbolic equilibrium $(0, 0)$ of the equivalent autonomous system

$$\begin{aligned} \frac{du_1}{dx} &= u_2 \\ \frac{du_2}{dx} &= \frac{au_1}{1 + bu_1}, \end{aligned} \quad (25)$$

where

$$u_1 = u \text{ and } u_2 = u',$$

is a saddle-point. Equation (24) is also equivalent to the conservation law

$$H \equiv H[u'(x), u(x)] := \frac{1}{2} \left(\frac{du}{dx} \right)^2 + K(u) = \text{constant}. \quad (26)$$

Here, H is the Hamiltonian of the system and

$$K(u) = \begin{cases} -a \left(\frac{bu - \ln(1+bu)}{b^2} \right) & \text{if } b > 0 \\ -\frac{au^2}{2} & \text{if } b = 0 \end{cases}. \quad (27)$$

With $x_m = m\Delta x$ ($m \in \mathbb{Z}$, $\Delta x > 0$) being the space node points and u_m an approximation of u at the point $x = x_m$, the linear equation

$$\frac{d^2 \underline{u}}{dx^2} - a\underline{u} = 0, \quad (28)$$

has the exact scheme (see [5])

$$\frac{\underline{u}_{m+1} - 2\underline{u}_m + \underline{u}_{m-1}}{\psi(\Delta x)^2} - a\underline{u}_m = 0, \quad (29)$$

where

$$\psi(\Delta x) = \frac{2}{\rho} \sinh\left(\frac{\rho\Delta x}{2}\right), \quad \rho = \sqrt{a}. \quad (30)$$

We follow the methodology in [18, 17] to consider, for (24), the NSFD scheme

$$\frac{u_{m+1} - 2u_m + u_{m-1}}{\psi(\Delta x)^2} - a \left(\frac{b(u_{m+1} - u_{m-1}) - \ln(1+bu_{m+1}) + \ln(1+bu_{m-1})}{b^2(u_{m+1} - u_{m-1})} \right) = 0, \quad (31)$$

where, by the mean-value theorem, we take

$$\frac{b(u_{m+1} - u_{m-1}) - [\ln(1+bu_{m+1}) - \ln(1+bu_{m-1})]}{b^2(u_{m+1} - u_{m-1})} = \frac{u_m}{1+bu_m} \text{ if } u_{m+1} = u_{m-1} \text{ or } b = 0. \quad (32)$$

Note that

$$\frac{b(u_{m+1} - u_{m-1}) - \ln(1+bu_{m+1}) + \ln(1+bu_{m-1})}{b^2(u_{m+1} - u_{m-1})} \geq 0,$$

by again the mean-value theorem, since

$$\frac{d[bu - \ln(1+bu)]}{du} = \frac{b^2 u}{1+bu} \geq 0 \text{ for } u \geq 0.$$

The underlying point of the NSFD scheme (31) is its equivalence to a discrete analogue of the conservation law (26). More precisely, we have the relation

$$\frac{1}{2} \left(\frac{u_{m+1} - u_m}{\psi(\Delta x)} \right)^2 + K_{\Delta x}(u_m) = \frac{1}{2} \left(\frac{u_m - u_{m-1}}{\psi(\Delta x)} \right)^2 + K_{\Delta x}(u_{m-1}), \quad (33)$$

where $K_{\Delta x}(u_m)$, with an initial guess $K_{\Delta x}(u_0)$, is derived from the identity

$$K_{\Delta x}(u_m) = K_{\Delta x}(u_{m-1}) + \frac{K(u_{m+1}) - K(u_{m-1})}{2}.$$

For instance if $K_{\Delta x}(u_0) = 0$, we have

$$K_{\Delta x}(u_m) = \begin{cases} \sum_{i=1}^m \frac{K(u_{i-1}) - K(u_{i-1})}{2} = \frac{K(u_{m+1}) - K(u_0)}{2} & \text{for } m \geq 1 \\ \sum_{i=1}^{|m|} \frac{K(u_{m-1+i}) - K(u_{m+1+i})}{2} & \text{if } m < 0. \end{cases} \quad (34)$$

We will not consider the numerical implementation of the NSFD scheme (31) and of its equivalent formulation (33), since this is done, for instance, in [17, 19] for similar discrete conservative systems,

where Mickens' rule on the nonlocal approximation of nonlinear terms is essential. Furthermore, the NSFD scheme (31) is equivalent to the system of difference equations

$$\begin{cases} \frac{u_{1,m+1} - u_{1,m}}{\psi(\Delta x)} = u_{2,m+1} \\ \frac{u_{2,m+1} - u_{2,m}}{\psi(\Delta x)} = a \left(\frac{b(u_{1,m+1} - u_{1,m-1}) - [\ln(1 + bu_{1,m+1}) - \ln(1 + bu_{1,m-1})]}{b^2(u_{1,m+1} - u_{1,m-1})} \right), \end{cases} \quad (35)$$

which, as a discrete analogue of the system (25), is an elementary stable NSFD scheme because the scheme reduces to the exact scheme (29) when $b = 0$. Since our primary focus is not on the replication of the conservation law (26), we shall also consider the NSFD scheme

$$\frac{u_{m+1} - 2u_m + u_{m-1}}{\psi(\Delta x)^2} - a \frac{u_m}{1 + bu_m} = 0,$$

which, though not preserving this property because of the violation of Mickens' rule on the nonlocal approximation of nonlinear terms, corresponds to an elementary stable NSFD scheme of the form similar to (35).

5 The M-M PDE

The reaction diffusion equation with the M-M term is

$$\frac{\partial u}{\partial t} = -\frac{au}{1 + bu} + \frac{\partial^2 u}{\partial x^2}. \quad (36)$$

Its comparison equation or its linearized equation about the equilibrium solution $\tilde{u} = 0$ is the classical linear parabolic equation

$$\frac{\partial u}{\partial t} = -au + \frac{\partial^2 u}{\partial x^2}. \quad (37)$$

We consider the same initial function $u^0(x)$ for the problems (36) and (37):

$$u(0, x) = u^0(x) = \underline{u}(0, x). \quad (38)$$

The real-valued function $u \rightarrow \frac{au}{1 + bu}$ satisfies $\frac{au}{1 + bu} \leq au$ on \mathbb{R}_+ and has bounded derivative $u \mapsto \frac{a}{(1 + bu)^2}$ on \mathbb{R}_+ . On the other hand, the Sturm-Liouville problem defined by the operator in the right-hand side of (37), with boundary conditions $\phi(0) = \phi(1) = 0$, has eigenvalues and associated (L^2 -orthonormal) eigenfunctions

$$\lambda_n = -a - n^2\pi^2 \text{ and } \phi_n(x) = 2 \sin(n\pi x), \quad n = 1, 2, \dots,$$

respectively. Thus, the standard existence, uniqueness, comparison and stability results (see for example [20, 21]) apply to the problem (36), as specified in the next theorem.

Theorem 6 *For a given bounded and continuous function $u^0(x)$, the initial value problems (36), (37) and (38) admit unique solutions $u(t, x)$ and $\underline{u}(t, x)$ such that*

$$0 \leq u^0(x) \implies 0 \leq \underline{u}(t, x) \leq u(t, x) \leq M := \sup_x u^0(x). \quad (39)$$

The equilibrium solution $\tilde{u} = 0$ of (36) and (38) is L^∞ asymptotically stable. Furthermore, if the initial-value problem is coupled with the Dirichlet boundary condition $u(t, 0) = u(t, 1) = 0$, then the equilibrium solution $\tilde{u} = 0$ is L^2 asymptotically stable in the precise manner that the kinetic energy

$$E(u(t)) := \frac{1}{2} \int_0^1 |u(t, x)|^2 dx, \quad (40)$$

decreases monotonically to 0 as $t \rightarrow \infty$.

Our aim is to consider for (36) various NSFD schemes and to demonstrate theoretically and computationally that they are dynamically consistent with the property (39). The stability properties will be demonstrated computationally. The general strategy, which strictly speaking makes sense when the so-called ‘‘lumped parameter assumption’’[21] is valid, consists in suitably combining the space-independent NSFD schemes in Sect. 3 with the time-independent schemes in Sect. 4.

Firstly, we deal with the schemes (17), (19), (4) and (31) to obtain the following explicit NSFD schemes, respectively:

$$\frac{u_m^{k+1} - u_m^k}{\phi_1(\Delta t)} = -\frac{au_m^{k+1}}{1 + bu_m^k} + \frac{u_{m+1}^k - 2u_m^k + u_{m-1}^k}{\psi(\Delta x)^2}, \quad (41)$$

and

$$\begin{aligned} \frac{u_m^{k+1} - u_m^k}{\phi_1(\Delta t)} &= -a \frac{u_m^{k+1}}{u_m^k} \left(\frac{b(u_{m+1}^k - u_{m-1}^k) - \ln(1 + bu_{m+1}^k) + \ln(1 + bu_{m-1}^k)}{b^2(u_{m+1}^k - u_{m-1}^k)} \right) \\ &\quad + \frac{u_{m+1}^k - 2u_m^k + u_{m-1}^k}{\psi(\Delta x)^2}, \end{aligned} \quad (42)$$

$$\frac{u_m^{k+1} - u_m^k}{\phi_2(\Delta t)} = -\frac{au_m^k}{1 + bu_m^k} + \frac{u_{m+1}^k - 2u_m^k + u_{m-1}^k}{\psi(\Delta x)^2}, \quad (43)$$

and

$$\begin{aligned} \frac{u_m^{k+1} - u_m^k}{\phi_2(\Delta t)} &= -a \left(\frac{b(u_{m+1}^k - u_{m-1}^k) - \ln(1 + bu_{m+1}^k) + \ln(1 + bu_{m-1}^k)}{b^2(u_{m+1}^k - u_{m-1}^k)} \right) \\ &\quad + \frac{u_{m+1}^k - 2u_m^k + u_{m-1}^k}{\psi(\Delta x)^2}. \end{aligned} \quad (44)$$

Secondly, we are interested in combining the exact scheme (16) with (4) to obtain the explicit NSFD scheme

$$\frac{u_m^{k+1} - u_m^k}{\phi_2(\Delta t)} = \frac{W((b \exp(-a\Delta t)u_m^k \exp(bu_m^k)) - bu_m^k)}{b\phi_2(\Delta t)} + \frac{u_{m+1}^k - 2u_m^k + u_{m-1}^k}{\psi(\Delta x)^2}. \quad (45)$$

In terms of the Lambert W -function, the following explicit NSFD scheme, which is tailored from the scheme (42) and (45), preserves the conservation law in the stationary case:

$$\begin{aligned} \frac{u_m^{k+1} - u_m^k}{\phi_2(\Delta t)} &= -a \frac{u_m^{k+1}}{u_m^k} \left\{ \frac{1}{b} + \frac{-\ln[1 + W((b \exp(-a\Delta t)u_{m+1}^k \exp(bu_{m+1}^k))] + \ln(1 + bu_{m-1}^k)}{b[W((b \exp(-a\Delta t)u_{m+1}^k \exp(bu_{m+1}^k)) - bu_{m-1}^k]} \right\} \\ &\quad + \frac{u_{m+1}^k - 2u_m^k + u_{m-1}^k}{\psi(\Delta x)^2}. \end{aligned} \quad (46)$$

Notice that both NSFD schemes (45) and (46) can, in view of the mean-value theorem, reduce to:

$$\frac{u_m^{k+1} - u_m^k}{\phi_2(\Delta t)} = -a \frac{u_m^{k+1}}{1 + bu_m^k} + \frac{u_{m+1}^k - 2u_m^k + u_{m-1}^k}{\psi(\Delta x)^2}. \quad (47)$$

As observed first by Mickens [22], the next result confirms the relevance of a functional relation between step sizes in order for an explicit NSFD scheme to preserve the positivity and boundedness property.

Theorem 7 *Assume that $\psi(\Delta x)$ is chosen such that the functional relation*

$$\frac{\phi_i(\Delta t)}{\psi(\Delta x)^2} = \frac{1}{2} \quad (48)$$

occurs between the step sizes. Then, we have the following positivity and boundedness property for the explicit NSFD schemes (41) and (42), (43) and (44), (45) and (46):

$$0 \leq u_m^0 \leq M \implies 0 \leq \underline{u}_m^k \leq u_m^k \leq M, \quad \forall k \geq 0, \forall m \in \mathbb{Z}, \text{ and } S^k \downarrow 0 \text{ as } k \rightarrow \infty$$

Here, \underline{u}_m^k denotes the discrete solution for the equation (37), resulting on setting $b = 0$ in each one of the above-mentioned NSFD schemes and $S^k := \sup_m u_m^k$.

Proof. Observe first that (48) is similar to a typical condition of Lax-Richtmyer stability of the involved explicit finite difference schemes for the linear equation (37) (see e.g. [23]). This condition allows us to re-write each one of the above NSFD schemes in the compact form

$$\begin{aligned} u_m^{k+1} &= \frac{u_{m+1}^k + u_{m-1}^k}{2[1 + g(b)]} \\ \underline{u}_m^{k+1} &= \frac{\underline{u}_{m+1}^k + \underline{u}_{m-1}^k}{2[1 + g(0)]} \end{aligned}$$

for some function g satisfying

$$g(0) \geq g(b) \geq 0.$$

This implies that (S^k) and (\underline{S}^k) are nonnegative monotonic decreasing sequences such that

$$S^k \downarrow 0 \text{ as } k \rightarrow \infty$$

and by mathematical induction on k , we have

$$0 \leq \underline{u}_m^k \leq u_m^k \leq M.$$

■

Remark 8 We will not investigate the combination of (18) with (4) and (31), which leads to the following implicit NSFD schemes that are not easy to solve in u_m^{k+1} :

$$\frac{u_m^{k+1} - u_m^k}{\phi_1(\Delta t)} = -\frac{au_m^{k+1}}{1 + bu_m^{k+1}} + \frac{u_{m+1}^k - 2u_m^k + u_{m-1}^k}{\psi(\Delta x)^2}. \quad (49)$$

and

$$\begin{aligned} \frac{u_m^{k+1} - u_m^k}{\phi_1(\Delta t)} &= -a \left(\frac{b(u_{m+1}^{k+1} - u_{m-1}^{k+1}) - \ln(1 + bu_{m+1}^{k+1}) + \ln(1 + bu_{m-1}^{k+1})}{b^2(u_{m+1}^{k+1} - u_{m-1}^{k+1})} \right) \\ &\quad + \frac{u_{m+1}^k - 2u_m^k + u_{m-1}^k}{\psi(\Delta x)^2}. \end{aligned} \quad (50)$$

As far as the positivity of discrete solutions is concerned, it is possible to achieve it by considering implicit NSFD schemes in which $(\Delta x)^2$ is used in place of $\psi(\Delta x)^2$ and the condition (48) is not needed. The precise result reads as follows:

Theorem 9 Assume that Dirichlet boundary conditions are prescribed for the problem (36), namely

$$u(t, -p) = \alpha \text{ and } u(t, p) = \beta,$$

(with $p > 0$, $\alpha \geq 0$ and $\beta \geq 0$) so that a finite number of nodes $x_m = m\Delta x$, $m = 0, \pm 1, \dots, \pm N$, are considered where $N \geq 2$ is an integer and $\Delta x = p/N$. Then the positivity of the solutions of (36) and of the comparison equation (37) is preserved by all the implicit NSFD schemes obtained from (41), (42), (43), (44), (45) and (46) by replacing

$$\frac{u_{m+1}^k - 2u_m^k + u_{m-1}^k}{\psi(\Delta x)^2} \text{ with } \frac{u_{m+1}^{k+1} - 2u_m^{k+1} + u_{m-1}^{k+1}}{(\Delta x)^2}. \quad (51)$$

Proof. To be specific, we focus only on the following implicit NSFD scheme obtained from (41), although the analysis below applies to all of them:

$$\frac{u_m^{k+1} - u_m^k}{\phi_1(\Delta t)} = -\frac{au_m^{k+1}}{1 + bu_m^k} + \frac{u_{m+1}^{k+1} - 2u_m^{k+1} + u_{m-1}^{k+1}}{(\Delta x)^2}. \quad (52)$$

Consider the column vector

$$U^{k+1} = [u_{-N+1}^{k+1} \cdots u_m^{k+1} \cdots u_{N-1}^{k+1}]^T.$$

Then the method (52) is equivalent to solving at each step the algebraic linear system

$$A_b U^{k+1} = F^k \quad (53)$$

where

$$A_b = \begin{bmatrix} 1 + 2c + \frac{a\phi_1(\Delta t)}{1+bu_{1-N}^k} & -c & 0 \cdots & 0 \\ -c & 1 + 2c + \frac{a\phi_1(\Delta t)}{1+bu_{2-N}^k} & -c \cdots & 0 \\ 0 & -c & 1 + 2c + \frac{a\phi_1(\Delta t)}{1+bu_{3-N}^k} \cdots & 0 \\ \vdots & \vdots & \vdots & \vdots \\ 0 & 0 & 0 \cdots & -c \quad 1 + 2c + \frac{a\phi_1(\Delta t)}{1+bu_{N-1}^k} \end{bmatrix}$$

$$c = \frac{\phi_1(\Delta t)}{(\Delta x)^2}$$

and

$$F^k = [u_{-N+1}^k + \alpha c, u_{-N+2}^k \cdots, u_{N-2}^k, u_{N-1}^k + \beta c]^T.$$

The tridiagonal matrix A_b is an M -matrix, being a strictly diagonally dominant matrix with positive diagonal and non-positive off diagonal [25]. Thus

$$U^k \geq 0 \implies U^{k+1} = A_b^{-1} F^k \geq 0.$$

Furthermore, since $A_b \leq A_0$, we have [26]

$$0 \leq \underline{U}^1 = A_0^{-1} F^0 \leq A_b^{-1} F^0 = U^1,$$

which by mathematical induction yields

$$0 \leq \underline{U}^k \leq U^k.$$

■

6 The M-M advection reaction equation

The advection equation with a M-M reaction term is

$$\frac{\partial u}{\partial t} + d \frac{\partial u}{\partial x} = -\frac{au}{1+bu}, \quad d > 0. \quad (54)$$

Considering separately the space and the time independent forms of (54), which are both of the type (3), it makes sense to combine suitably the NSFD schemes presented in Section 3. We obtain the numerical schemes

$$\begin{aligned} \frac{u_m^{k+1} - u_m^k}{\phi_1(\Delta t)} + d \frac{u_m^k - u_{m-1}^k}{d\phi_1(\Delta x/d)} &= -\frac{au_m^{k+1}}{1+bu_{m-1}^k}, \\ \frac{u_m^{k+1} - u_m^k}{\phi_2(\Delta t)} + d \frac{u_m^k - u_{m-1}^k}{d\phi_2(\Delta x/d)} &= -\frac{au_{m-1}^k}{1+bu_{m-1}^k}, \\ \frac{u_m^{k+1} - u_m^k}{\phi_2(\Delta t)} + d \frac{u_m^k - u_{m-1}^k}{d\phi_2(\Delta x/d)} &= \frac{W((b \exp(-a\Delta t)u_{m-1}^k \exp(bu_{m-1}^k)) - bu_{m-1}^k)}{b\phi_2(\Delta t)}, \end{aligned} \quad (55)$$

which, on requiring the functional relation

$$\phi_i(\Delta t) = \phi_i(d^{-1}\Delta x) \text{ i.e. } \Delta x = d\Delta t, \quad i = 1, 2, \quad (56)$$

reduce to the following NSFD schemes:

$$\frac{u_m^{k+1} - u_{m-1}^k}{\phi_1(\Delta t)} = -\frac{au_m^{k+1}}{1+bu_{m-1}^k}, \quad (57)$$

$$\frac{u_m^{k+1} - u_{m-1}^k}{\phi_2(\Delta t)} = -\frac{au_{m-1}^k}{1 + bu_{m-1}^k}, \quad (58)$$

and

$$\frac{u_m^{k+1} - u_{m-1}^k}{\phi_2(\Delta t)} = \frac{W((b \exp(-a\Delta t)u_{m-1}^k \exp(bu_{m-1}^k)) - bu_{m-1}^k)}{b\phi_2(\Delta t)}. \quad (59)$$

Observe that the schemes (57), (58) and (59) depend only on u_m^{k+1} and u_{m-1}^k , in accordance with a general result obtained by Mickens [24] for the PDE

$$\frac{\partial u}{\partial t} + d \frac{\partial u}{\partial x} = f(u).$$

The reason for this is that the solutions should only move along the characteristics and, in fact along the characteristics, the advection-reaction equation (54) becomes, for a fixed $x \in \mathbb{R}$, the M-M ODE:

$$\frac{dU}{dt} = -\frac{aU}{1 + bU}, \quad (60)$$

where

$$t \rightarrow t, \quad x \rightarrow x + dt, \quad U(t) := u(t, x + dt). \quad (61)$$

Note that Eq. (54) is just Eq. (3) with a linear advection term. It may be compared to

$$\frac{\partial u}{\partial t} + d \frac{\partial u}{\partial x} = -au$$

to examine the existence, boundedness and other solution properties. Also, in view of the connection with the M-M ODE (60), the properties of the solutions of (54) along the characteristics are similar to those stated in Theorem 1. In the next theorem, we state how some of these properties are preserved by the NSFD schemes (57), (58) and (59) along the lines of Theorems 3 and 7.

Theorem 10 *Under the relation (56), we have*

$$0 \leq u_m^0 \leq M \implies 0 \leq u_m^k \leq M, \forall k \geq 0, \forall m \in \mathbb{Z}, \text{ and } S^k \downarrow 0 \text{ as } k \rightarrow \infty.$$

Proof. For a fixed space grid point x_{m-k} , we have $x_{m-k} = x_m - dt_k$ by (56). The assumption on the initial values in the theorem implies that $0 \leq u_{m-k}^0 \leq M$ which, for the function U associated with $x = x_{m-k}$ and given by (60)-(61), means that $0 \leq U^0 \leq M$. It follows from Theorem 3 and (61) that $0 \leq U^k \leq U^{k-1} \leq U^0 \leq M$ or $0 \leq u_m^k \leq u_{m-1}^{k-1} \leq u_{m-k}^0 \leq M$. Thus $0 \leq S^k \leq S^{k-1} \leq S^0 \leq M$ and $S^k \downarrow 0$. ■

7 The M-M advection reaction-diffusion equation

The advection-diffusion equation with a M-M reaction term is

$$\frac{\partial u}{\partial t} + d \frac{\partial u}{\partial x} = -\frac{au}{1 + bu} + \frac{\partial^2 u}{\partial x^2} \quad (62)$$

and the physical solutions should have the positivity property (39). In order to construct a scheme that preserves the property (39), it seems natural to combine the approach in Sections 5 and 6. However, this would require the imposition of conditions (48) and (56), which taken simultaneously are incompatible.

First, let us avoid the condition (48) and keep condition (56). Using (51), one possible NSFD scheme is

$$\frac{u_m^{k+1} - u_{m-1}^k}{\phi_2(\Delta t)} = \frac{W((b \exp(-a\Delta t)u_{m-1}^k \exp(bu_{m-1}^k)) - bu_{m-1}^k)}{b\phi_2(\Delta t)} + \frac{u_{m+1}^{k+1} - 2u_m^{k+1} + u_{m-1}^{k+1}}{(\Delta x)^2}. \quad (63)$$

Analogously to Theorem 9, if boundary conditions are specified, the NSFD scheme (63) reduces to a workable formulation similar to (53), with an M matrix such that the positivity property is preserved.

Secondly, we want to avoid both conditions (48) and (56). To this end, we follow an idea in [27, 28]. Given $x_m = m\Delta x$, we introduce

$$\bar{x}_m := x_m - d\Delta t$$

the backtrack point of x_m , which is not in general on the grid. For any x_m , there exists an integer m_1 such that

$$x_{m_1-1} < \bar{x}_m \leq x_{m_1}.$$

Using the linear Lagrange interpolation at the points $(x_{m_1-1}, u_{m_1-1}^k)$ and $(x_{m_1}, u_{m_1}^k)$, let us consider the following point on this line:

$$\bar{u}_m^k := \frac{\bar{x}_m - x_{m_1}}{-\Delta x} u_{m_1-1}^k + \frac{\bar{x}_m - x_{m_1-1}}{\Delta x} u_{m_1}^k.$$

Notice that $\bar{u}_m^k \geq 0$ if $u_{m_1-1}^k$ and $u_{m_1}^k$ are nonnegative. One possible NSFD scheme for (62) is

$$\frac{u_m^{k+1} - \bar{u}_m^k}{\phi_2(\Delta t)} = \frac{W((b \exp(-a\Delta t) \bar{u}_m^k \exp(b\bar{u}_m^k)) - b\bar{u}_m^k)}{b\phi_2(\Delta t)} + \frac{u_{m+1}^{k+1} - 2u_m^{k+1} + u_{m-1}^{k+1}}{(\Delta x)^2}, \quad (64)$$

which enjoys the same dynamic consistency properties as the scheme (63).

Finally, the explicit NSFD scheme

$$\frac{u_m^{k+1} - \bar{u}_m^k}{\phi_2(\Delta t)} = \frac{W((b \exp(-a\Delta t) \bar{u}_m^k \exp(b\bar{u}_m^k)) - b\bar{u}_m^k)}{b\phi_2(\Delta t)} + \frac{u_{m+1}^k - 2\bar{u}_m^k + u_{m-1}^k}{\psi(\Delta x)^2}, \quad (65)$$

can be used. The left-hand sides of (64) and (65) approximate the left-hand side of (62), following a rewriting similar to (55). In summary, we have the following result:

Theorem 11 *With suitable boundary conditions, the NSFD schemes (63) and (64) preserve the property (39). The same property is preserved by the NSFD scheme (65) under the relation (48).*

8 Numerical simulations

In this section, we demonstrate computationally the theoretical results obtained in the previous sections. The results confirm in particular that the NSFD schemes constructed by using Mickens' classical rules are reliable and thus they can be used when exact schemes are not available. We have purposely decided not comment too much on standard finite difference schemes, since their poor performance has been extensively reported in the literature (see, for instance, [17], [27], [5], [6] and [7]). In all the examples presented below, we take $a = 0.1$; the time step is $\Delta t = 2$, which is considered to be large for standard numerical schemes. In the simulation involving Lambert W function, we use the Matlab built-in function "lambertw(*)".

Figure 1 supports the theory in Theorem 3 and Remark 2. It is seen that the NSFD schemes (17), (18) and (19) perform as efficiently as the exact scheme (11) or (16) regarding the preservation of the dynamics of the system stated in Theorem 1 when $b = 1$ and $b = 0$, respectively. Among other things, the same figure displays the global asymptotic stability of the equilibrium solution $\tilde{u} = 0$ given in Remark 4. The contrast with the standard scheme (23) and the Matlab ODE45 solver is visualized in Figure 2. The apparent good results by the ODE45 solver are at the high cost of very small time steps Δt , which is a serious concern when one is interested in the long term behavior of the solution, or for stiff/chaotic problems, [19].

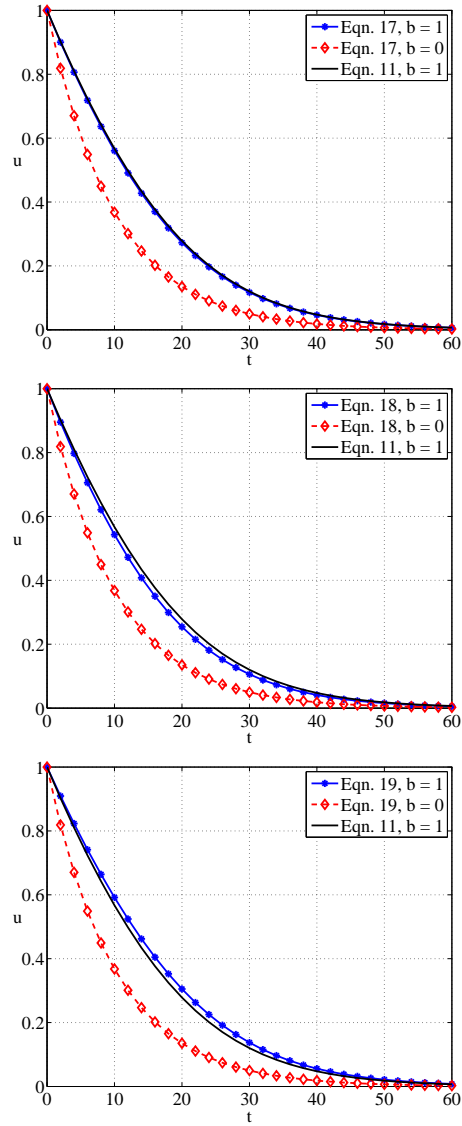
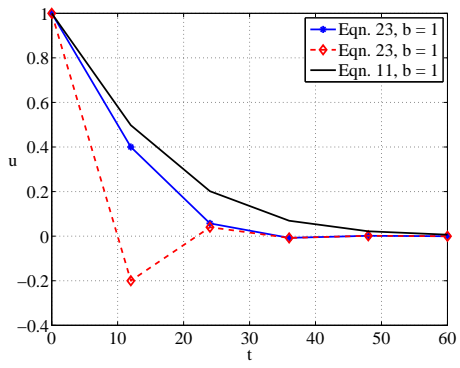
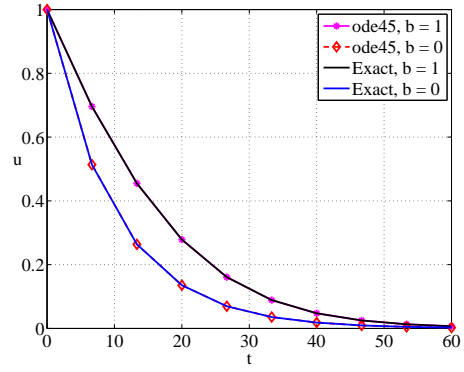


Figure 1: NSFD schemes (17), (18) and (19) versus the exact scheme (11)



(a).



(b).

Figure 2: Standard scheme (23) in (a) and ODE45 Solver in (b).

Figures 3, 6, 7 and 8 illustrate Theorem 7 for the explicit NSFD schemes (41), (42), (43) and (44), respectively. The initial function is $u^0(x) = e^{-x^2}$, $x \in \mathbb{R}$. The value of the space size Δx is obtained according to (48), i.e. $\psi(\Delta x) = \sqrt{2\phi_i(\Delta t)} = \sqrt{2\phi_i(2)}$, where $i = 1, 2$, while we take $b = 1$ and $b = 0$. It is seen on the pictures that the NSFD schemes compare nicely with the exact scheme-related method (45), as far as the replication of the properties in Theorem 6 is concerned. This includes the stated L^∞ -stability of the equilibrium solution $\tilde{u} = 0$, while the decay to 0 of the kinetic energy is displayed on Figure 5 (a). The poor performance of the standard finite difference method is shown on Figure 4, which exhibits negative solutions, and Figure 5 (b). Here and after, the associated Figure (a) shows, in each case, a side-view profile corresponding to Figure (b) taken at $x = 0$. The excellence performance of the NSFD schemes is further confirmed by the values of the solutions tabulated in Tables 1, 2, 3 and 4.

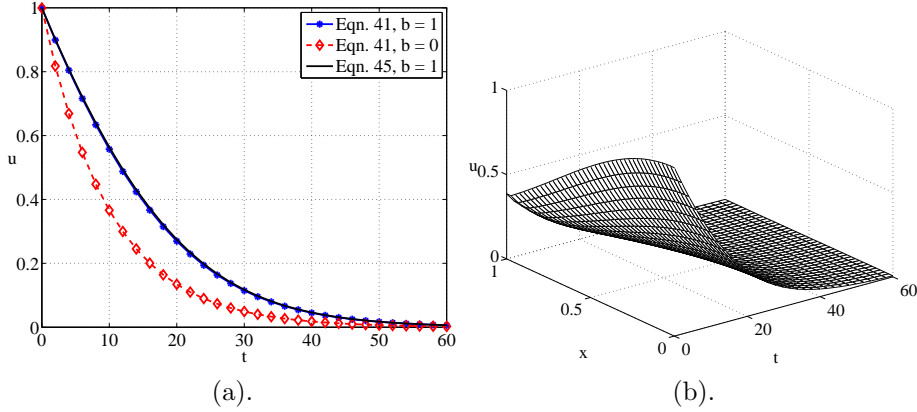


Figure 3: NSFD scheme (41) versus the exact scheme-related method (45).

t	x	\underline{u}	u	Exact
0	0	1.0000	1.0000	1.0000
10	0.1667	0.3611	0.5475	0.5537
20	0.3333	0.1264	0.2459	0.2504
30	0.5000	0.0430	0.0911	0.0929
40	0.6667	0.0142	0.0295	0.0300
50	0.8333	0.0045	0.0088	0.0089
60	1.0000	0.0014	0.0025	0.0010

Table 1: Comparative results corresponding to Figure 3

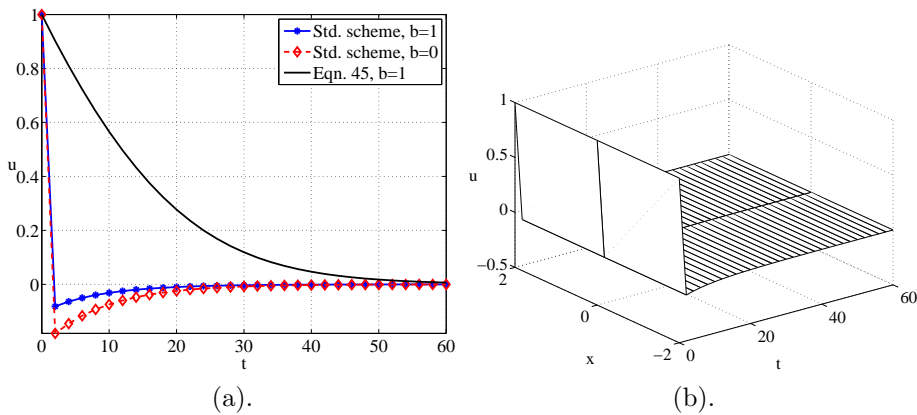
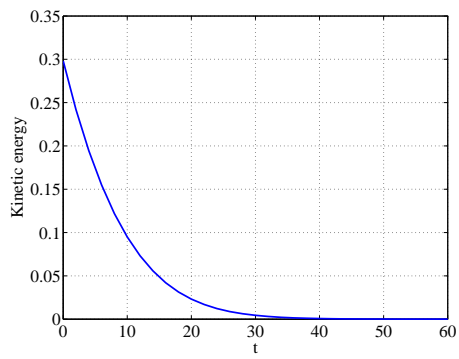
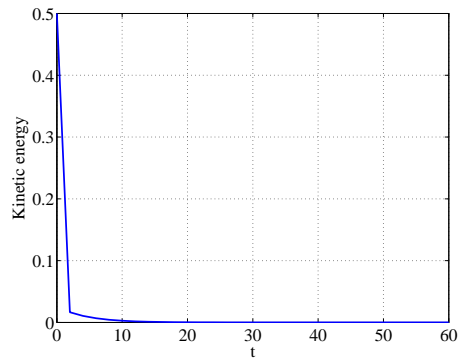


Figure 4: Standard scheme corresponding to (43) for $\phi_i(\Delta t) = \Delta t = 2$, $\psi(\Delta x) = \Delta x = 2$.



(a).



(b).

Figure 5: Kinetic energy profiles for: (a) NSFD scheme (43) and, (b) the standard finite difference scheme related to (43) for $\phi_i(\Delta t) = \Delta t$, $\psi(\Delta x) = \Delta x$.

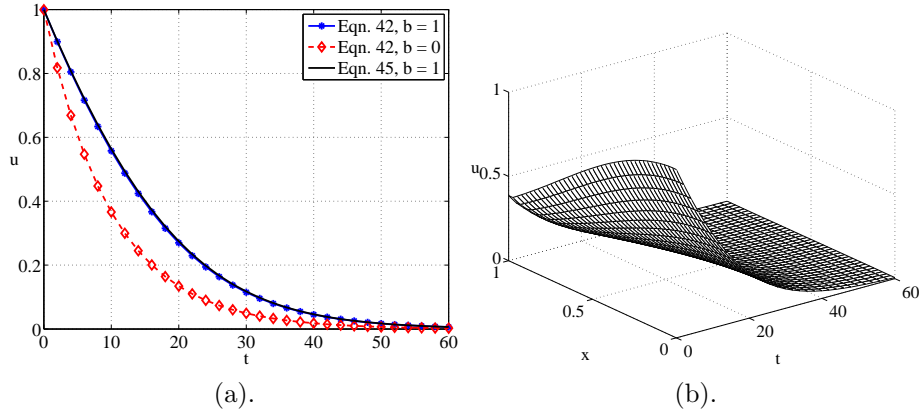


Figure 6: NSFD scheme (42) versus the exact scheme-related method (45).

t	x	\underline{u}	u	Exact
0	0	1.0000	1.0000	1.0000
10	0.1667	0.3611	0.5477	0.5537
20	0.3333	0.1264	0.2461	0.2504
30	0.5000	0.0430	0.0912	0.0929
40	0.6667	0.0142	0.0295	0.0300
50	0.8333	0.0045	0.0088	0.0089
60	1.0000	0.0014	0.0025	0.0010

Table 2: Comparative results corresponding to Figure 6

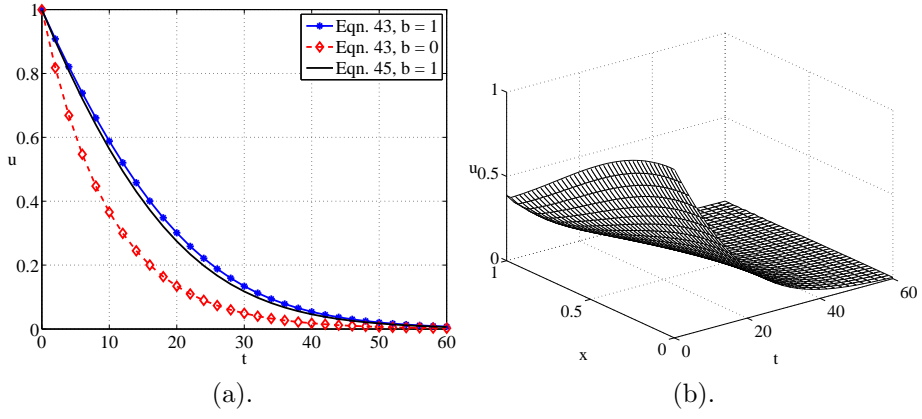


Figure 7: NSFD scheme (43) versus the exact scheme-related method (45).

t	x	\underline{u}	u	Exact
0	0	1.0000	1.0000	1.0000
10	0.1667	0.3608	0.5777	0.5537
20	0.3333	0.1263	0.2741	0.2504
30	0.5000	0.0429	0.1052	0.0929
40	0.6667	0.0142	0.0343	0.0300
50	0.8333	0.0045	0.0101	0.0089
60	1.0000	0.0010	0.0015	0.0010

Table 3: Comparative results corresponding to Figure 7

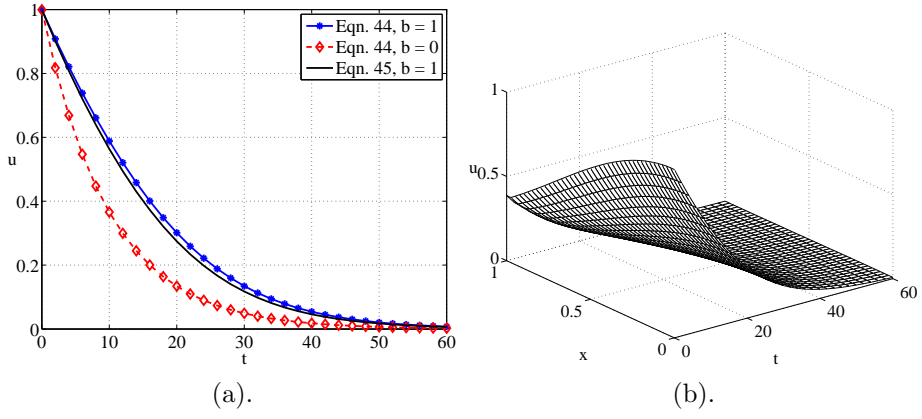


Figure 8: NSFD scheme (44) versus the exact scheme-related method (45).

t	x	\underline{u}	u	Exact
0	0	1.0000	1.0000	1.0000
10	0.1667	0.3608	0.5778	0.5537
20	0.3333	0.1263	0.2743	0.2504
30	0.5000	0.0429	0.1053	0.0929
40	0.6667	0.0142	0.0343	0.0300
50	0.8333	0.0045	0.0102	0.0089
60	1.0000	0.0010	0.0029	0.0010

Table 4: Comparative results corresponding to Figure 8

Mike: we should add two figures: one on the decay of the kinetic energy and another one on standard finite difference method.

Figure 9 illustrates Theorem 9 for the preservation of the positivity of solutions when the implicit NSFD scheme (52) is used. From now on, the standard scheme is no longer plotted due to its poor performance mentioned and observed above. We take $p = 1$ and consider homogenous Dirichlet boundary conditions i.e. $\alpha = \beta = 0$. The initial value is $u^0(x) = |\sin \pi x|$ for $x \in [-1, 1]$ and $u^0(x) = 0$ for $|x| > 1$. The space step size is $\Delta x = 0.1$, which varies independently from $\Delta t = 2$ in the sense that the requirement (48) is not met. Apart from the positivity of the discrete solutions, Table 5 confirms the expected comparison between the solutions u_m^k for $b = 1$ and \underline{u}_m^k for $b = 0$.

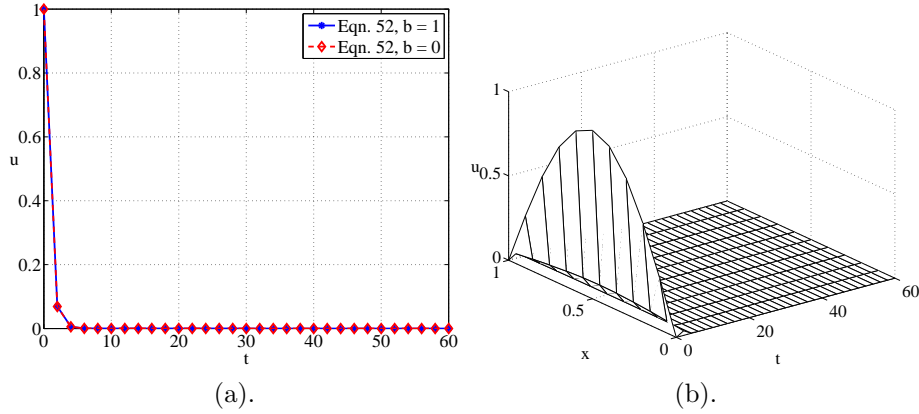


Figure 9: Positivity of the implicit NSFD scheme(52).

t	x	\underline{u}	u
0	0	3.090×10^{-1}	3.090×10^{-1}
10	0.1667	1.255×10^{-6}	1.265×10^{-6}
20	0.3333	6.344×10^{-12}	6.398×10^{-12}
30	0.5000	2.799×10^{-16}	2.822×10^{-17}
40	0.6667	1.135×10^{-22}	1.144×10^{-22}
50	0.8333	4.321×10^{-28}	4.357×10^{-28}
60	1.0000	1.559×10^{-33}	1.572×10^{-33}

Table 5: Comparative results corresponding to Figure 9

Figures 10 and 11 illustrate the positivity and boundedness property in Theorem 10 for the explicit NSFD schemes (57) and (58) with initial value $u^0(x) = e^{-x^2}$, $x \in \mathbb{R}$. With $d = 0.1$ and $b = 1$, we take the space step size in accordance with (56), i.e. $\Delta x = 0.2$. The results compare nicely with the exact scheme-related method (59), as also shown on Tables 6 and 7.

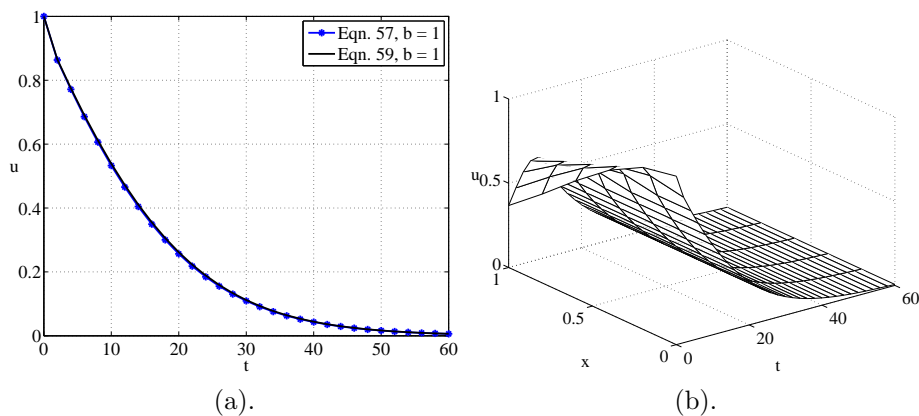


Figure 10: Positivity and boundedness of the NSFD scheme (57) versus the exact scheme-related method (59).

t	x	u	Exact
0	0	1.0000	1.0000
10	0.1667	0.5328	0.5389
20	0.3333	0.2565	0.2616
30	0.5000	0.1091	0.1118
40	0.6667	0.0429	0.0440
50	0.8333	0.0162	0.0166
60	1.0000	0.0060	0.0062

Table 6: Comparative results corresponding to Figure 10

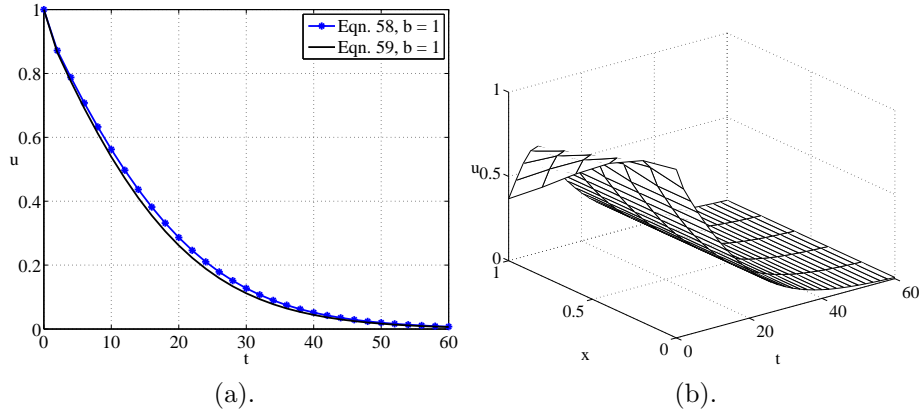


Figure 11: Positivity and boundedness of the NSFD scheme (58) versus the exact scheme-related method (59).

t	x	u	Exact
0	0	1.0000	1.0000
10	0.1667	0.5623	0.5389
20	0.3333	0.2865	0.2616
30	0.5000	0.1275	0.1118
40	0.6667	0.0514	0.0440
50	0.8333	0.0197	0.0166
60	1.0000	0.0073	0.0062

Table 7: Comparative results corresponding to Figure 11

Finally, Figure 12 illustrates the positivity of solutions in Theorem 11 for the scheme (65) for the initial condition $u^0(x) = e^{-x^2}$, $b = 1$, $d = 0.1$ and Δx obtained according to (48) i.e. $\psi(\Delta x) = \sqrt{2\phi_2(2)}$.

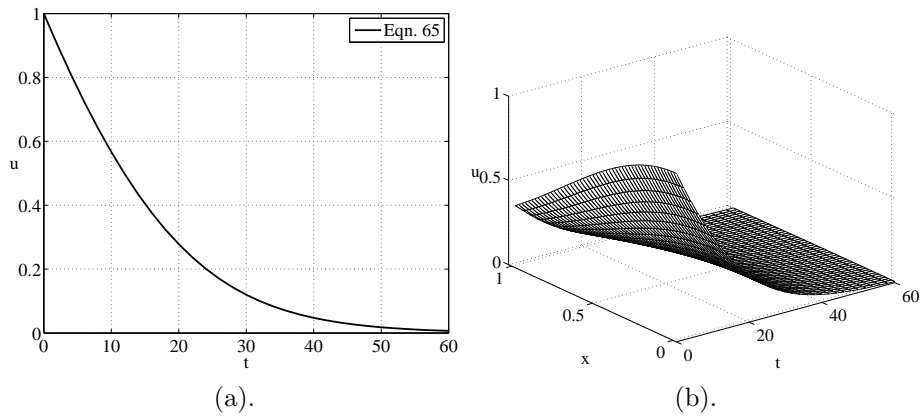


Figure 12: Positivity of the NSFD scheme (65).

9 Conclusion

This paper is motivated by the exact scheme of the Michaelis-Menten ordinary differential equation designed recently in [8]. Using Mickens' rules [5] and the specific form of the right-hand side of the M-M equation, we introduced several new NSFD schemes for the M-M equation as well as for associated reaction-diffusion-type equations. We demonstrated theoretically and computationally that the new NSFD schemes are dynamically consistent with the continuous model. They all perform as efficiently as the exact scheme and exact-related methods, confirming thus the power of the nonstandard approach.

Our future interest is on the application of the results of this study to the design of NSFD schemes for epidemiological models where the contact between the susceptible individuals $S(t)$, and the infected individuals $I(t)$, in the total population $N(t)$, is expressed by a nonlinear term of the form $\frac{S(t)I(t)}{N(t)}$, which is similar to that of the M-M equation (see [29]). Preliminary work in this direction is done in [30]. Furthermore, we are investigating how the study could be extended to the combustion model $\frac{du}{dt} = u^2(1-u)$ whose exact scheme can be deduced from [9] as

$$u^{k+1} = \{1 + W[(u^k - 1)^{-1} \exp((u^k - 1)^{-1} - \Delta t)]\}^{-1}.$$

Acknowledgments

The work was initiated when JM-SL was on sabbatical leave at Clark Atlanta University in February 2009. JM-SL is grateful to the South African National Research Foundation for funding the visit as well as to R.E. Mickens and researchers in the Physics Department for making his visit the most pleasant and productive. We are also sincerely grateful to the anonymous reviewers whose comments have significantly improved this work.

References

- [1] R.E. O'Malley, Jr., *Singular perturbation methods for ordinary differential equations*, Springer-Verlag Applied Mathematical Sciences Series, New York, 1991.
- [2] L.A. Segel and M. Slemrod, The quasi-steady-state assumption: a case study in perturbation, *SIAM Review*, **31** (1989), 446–477.
- [3] D.T. Dimitrov and H.V. Kojouharov, Positive and elementary stable nonstandard numerical methods with applications to predator-prey models, *Journal of Computational and Applied Mathematics*, **189** (2006), 98–108.
- [4] D.T. Dimitrov and H.V. Kojouharov, Nonstandard numerical methods for a class of predator-prey models with predator interference, Proceedings of the 6th Mississippi State-UBA Conference on Differential Equations and Computational Simulations, 67–75, *Electronic Journal of Differential Equations Conference*, **15**, Southwest Texas State University, San Marco, 2007.
- [5] R.E. Mickens, *Nonstandard finite difference models of differential equations*, World Scientific, Singapore, 1994.
- [6] R.E. Mickens (Ed.), *Applications of nonstandard finite difference schemes*, World Scientific, Singapore, 2000.
- [7] R.E. Mickens (Ed.), *Advances in the applications of nonstandard finite difference schemes*, World Scientific, Singapore, 2005.
- [8] R.E. Mickens, An exact discretization of the Michaelis-Menten type equations with applications, *Journal of Biological Dynamics*, In press.
- [9] R.M. Corless, G.H. Gonnet, D.E.G. Hare, D.J. Jeffrey and D.E. Knuth, On the Lambert W function, *Advances in Computational Mathematics*, **5** (1996), 329–359.

- [10] R. Anguelov, J. M.-S. Lubuma, M. Shillor, Topological dynamic consistency of nonstandard finite difference schemes for dynamical systems, *Journal of Difference Equations and Applications*, **17** (2011), 1769–1791.
- [11] S. Schnell and P.K. Maini, Enzyme kinetics at high enzyme concentration, *Bulletin of Mathematical Biology*, **62** (2000), 483–499.
- [12] M. Abramowitz and I.A. Stegun (editors), *Handbook of mathematical functions with formulas, graphs and mathematical tables*, Dover Publications, New York, 9th edition, 1972.
- [13] W.H. Beyer (ed), *CRC standard mathematical tables*, 28th edition, 1987.
- [14] J.D. Murray, *Mathematical biology I: an introduction*, Springer, New York, 2002.
- [15] R.K. Miller, *Nonlinear Volterra integral equations*, Mathematics Lecture Note Series, W.A. Benjamin, Inc., Philippines, 1971.
- [16] W. Walter, *Differential and integral inequalities*, Springer-Verlag, Berlin, 1970.
- [17] R. Anguelov and J.M.-S. Lubuma, Contributions to the mathematics of the nonstandard finite difference method and applications, *Numerical Methods for Partial Differential Equations*, **17** (2001), 518-543.
- [18] R. Anguelov, P. Kama and J.M.-S. Lubuma, On non-standard finite difference models of reaction-diffusion equations, *Journal of Computational and Applied Mathematics*, **175** (2005) 11-29.
- [19] Y. Dumont and J.M.-S. Lubuma, Non-standard finite difference methods for vibro-impact problems, *Proceedings of the Royal Society of London Series A: Mathematical, Physical and Engineering Sciences*, **461A** (2005), 1927-1950.
- [20] J.D. Logan, *Nonlinear differential equations*, Wiley-Interscience, New York, 1994.
- [21] J. Smoller, *Shock waves and reaction diffusion equations*, Springer-Verlag, 1983.
- [22] R.E. Mickens, Relation between the time and space step-sizes in nonstandard finite-difference schemes for the Fisher equation, *Numerical Methods for Partial Differential Equations* **13** (1997), 51-55..
- [23] K.W. Morton and D.F. Mayers, *Numerical solutions of partial differential equations*, Cambridge University Press, London, 1994.
- [24] R. E. Mickens, Nonstandard finite difference scheme for scalar advection-reaction partial differential equations, *Neural, Parallel, and Scientific Computations*, **12** (2004), 163 - 174.
- [25] R.S. Varga, *Matrix iterative analysis*, Prentice-Hall, Englewood Cliffs, NJ, 1962.
- [26] A. Berman and R. J. Plemmons, *Nonnegative matrices in the mathematical sciences*, Academic Press, New York, 1979.
- [27] H.V. Kojouharov and B.M. Chen, Nonstandard methods for advection-diffusion-reaction equations, In: R.E. Mickens (Editor), *Applications of nonstandard finite difference schemes*, World Scientific, Singapore, 2000, pp. 55-108.
- [28] J.M-S Lubuma and K.C. Patidar, Solving singularly perturbed advection reaction equation via non-standard finite difference methods, *Mathematical Methods in the Applied Sciences*, **30** (2007), 1627-1637.
- [29] S.M. Garba, A.B Gumel and J.M.-S Lubuma, Dynamically-consistent nonstandard finite difference method for an epidemic model, *Mathematical and Computer Modeling*, **53** (2011), 131-150 (doi:10.1016/j.mcm.2010.07.026).
- [30] M. Chapwanya, J.M.-S Lubuma and R.E. Mickens, From Enzyme Kinetics to Epidemiological Models with Michaelis-Menten Contact Rate: Design of Nonstandard Finite Difference Schemes, *Computers and Mathematics with Applications*, 2012, in press, (doi:10.1016/j.camwa.2011.12.058).