From Enzyme Kinetics to Epidemiological Models with Michaelis-Menten Contact Rate: Design of Nonstandard Finite Difference Schemes

Michael Chapwanya[a], Jean M-S Lubuma[a,*], Ronald E Mickens[b]

[a]*Department of Mathematics and Applied Mathematics, University of Pretoria, Pretoria 0002 (South Africa)*
[b]*Department of Physics, Clark Atlanta University, Atlanta GA 30314 (USA)*

Abstract

We consider the basic SIR epidemiological model with the Michaelis-Menten formulation of the contact rate. From the study of Michaelis-Menten basic enzymatic reaction, we design two types of Nonstandard Finite Difference (NSFD) schemes for the SIR model: Exact-related schemes based on the Lambert W function and schemes obtained by using Mickens's rules of more complex denominator functions for discrete derivatives and nonlocal approximations of nonlinear terms. We compare and investigate the performance of the two types of schemes by showing that they are dynamically consistent with the continuous model. Numerical simulations that support the theory and demonstrate computationally the power of NSFD schemes are presented.

Keywords: nonstandard finite difference method, exact scheme, Lambert W function, Michaelis-Menten equation, SIR model, advection-reaction equations
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1. Introduction

One of the most basic enzymatic reaction was proposed more than a century ago by Michaelis and Menten. Following [1] in this introductory section, the process involves a substrate S that reacts with an enzyme E to form a complex ES which in turn is converted into a product P and the enzyme. This is represented schematically by

$$E + S \underset{k_{-1}}{\overset{k_1}{\rightleftharpoons}} ES \overset{k_2}{\longrightarrow} P + E,$$
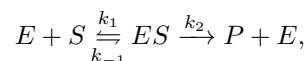
where k_1, k_{-1} and k_2 are positive constant parameters associated with the rates of reaction. Denoting, as usual in biochemistry, by $[X]$ the concentration of a reactant X, the mass action principle leads to the following model for this basic enzymatic reaction:

$$\frac{d[S]}{dt} = -k_1[E][S] + k_{-1}[ES], \tag{1}$$

$$\frac{d[E]}{dt} = -k_1[E][S] + (k_{-1} + k_2)[ES], \tag{2}$$

$$\frac{d[ES]}{dt} = k_1[E][S] - (k_{-1} + k_2)[ES], \tag{3}$$

$$\frac{d[P]}{dt} = k_2[ES]. \tag{4}$$

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*Corresponding author.
Email address: `jean.lubuma@up.ac.za` (Jean M-S Lubuma)

The system (1)-(4) is supplied with initial conditions:

$$[S](0) = [S]_0, \ [E](0) = [E]_0, \ [ES](0) = [ES]_0 \ \text{and} \ [P](0) = [P]_0. \tag{5}$$

In order to study the dynamics of the complex system (1)-(4), the tradition is to make the so-called Standard Quasi Steady -State Assumption (sQSSA). That is, at the initial stage of the complex $[ES]$, formation is very fast after which it is essentially at equilibrium i.e.,

$$\frac{d[ES]}{dt} \approx 0 \ \text{at the low enzyme concentration.} \tag{6}$$

Under the condition (6), the system (1)-(4) is reduced to the scalar equation

$$\frac{d[S]}{dt} = -\frac{k_2[E]_0[S]}{[S] + K_m}, \ [S](0) = [S]_0, \tag{7}$$

where $K_m = \dfrac{k_{-1} + k_2}{k_1}$ is called the Michaelis constant. Eq. (7) is the Michaelis-Menten (M-M) equation. It was also derived in [2] and [3] with a singular perturbation technique where $[S]$ is one of the leading order terms of the expansion of the outer solution. Since the enzyme is traditionally considered to be present in small amounts compared with the substrate, the assumption (6) that leads to (7) means that the substrate concentration effectively does not change during this initial transient stage. This is typically the case when the substrate concentration greatly exceeds that of the enzyme [4]:

$$\frac{[E]_0}{[S]_0} << 1. \tag{8}$$

On the contrary, at high enzyme concentration, the sQSSA or the assumption (6) is no longer valid. This well-known fact was recently comprehensibly analysed in [5] with the aid of the reverse Quasi-Steady State Assumption (rQSSA) where a necessary condition for its validity is the opposite of (8):

$$\frac{[E]_0}{[S]_0} >> 1. \tag{9}$$

In this case the following full system that results from the conservation law obtained by adding equations (2) and (3) must be used:

$$\frac{d[S]}{dt} = -k_1[E]_0[S] + (k_1[S] + k_{-1})[ES], \tag{10}$$

$$\frac{d[ES]}{dt} = k_1[E]_0[S] - (k_1[S] + k_{-1} + k_2)[ES]. \tag{11}$$

Despite the apparent simplification from (1)-(4) or (10)-(11) to (7), the solutions of the M-M equation cannot be found explicitly. Consequently, it is crucial to construct numerical methods which are reliable in that they provide useful information on the dynamics of the differential model. The particular type of information and properties on which many researchers have focused are the linear stability of the hyperbolic critical point $[\tilde{S}] = 0$ 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 (see the books [6], [7] and [8] and the references therein). In a recent work [9], which is based on the paper [10] on the exact scheme of the M-M equation via the so-called Lambert W function [11], the authors designed, for the M-M equation and major related reaction-partial differential equations, several innovative NSFD schemes that are dynamically consistent and sometimes topologically dynamically consistent in the sense of [12].

On the other hand, despite the restrictive validity of the equation (7) in the context of enzyme kinetics, its right-hand side is extensively used in ecological models of interacting populations and in epidemiology of

infectious diseases as a functional response, which captures well the fact that the number of contact made by an average invading or infective individual tends to saturate (see, for instance, [13], [14], [15], [16] and [17]). The purpose of the current work is primarily to explore how the study in [9] can be extended to epidemiological models. We restrict the analysis to the basic SIR model. We design, for this model, an exact scheme-related method and NSFD schemes that are obtained by using Mickens' rules [6]. One focus of the work is to compare and investigate the performance of these two types of numerical schemes.

The rest of the paper is organized as follows. In the next section, we study the M-M equation versus the decay equation, with the aim of emphasizing from their exact schemes that these equations have the same dynamics only near the critical point $[\tilde{S}] = 0$. Some of the NSFD schemes obtained in [9] are briefly discussed in Section 3, in preparation of Section 4 where new schemes are investigated for the SIR model. Section 5 provides concluding remarks pertaining to how the new NSFD schemes fit in the literature and how the study can be extended. As a matter of principle, numerical simulations that illustrate the power of NSFD schemes discussed in a given section are presented in the same section.

2. The M-M equation versus the decay equation

For convenience, the Michaelis-Menten (M-M) ordinary differential equation (7) is written as

$$\frac{du}{dt} = -\frac{au}{1 + bu}, \ a > 0, \ b \geq 0, \tag{12}$$

with initial condition

$$u(0) = u^0, \tag{13}$$

where $u = [S]$ is the concentration of the substrate S and the positive constant parameters are related by $\frac{a}{b} = k_2[E]_0$ and $\frac{1}{b} = K_m$ when $b > 0$. 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 [1]. The M-M equation (12) has only one fixed-point, namely $\tilde{u} = 0$. This fixed-point is hyperbolic since the derivative of the right-hand at $\tilde{u} = 0$ is different from 0, i.e.,

$$\left(-\frac{au}{1 + bu} \right)' = -\frac{a}{(1 + bu)^2}. \tag{14}$$

Consequently, the Hartman-Grobman theorem [18] is valid. Near the fixed-point $\tilde{u} = 0$, the M-M equation has the same asymptotic behavior as the decay equation

$$\frac{d\underline{u}}{dt} = -a\underline{u}, \ a > 0, \tag{15}$$

which is its linearized form about this fixed point. More so, due to the negative sign in (14), the fixed-point $\tilde{u} = 0$ is globally asymptotically stable. This result explains why the study of the M-M equation has been extensively replaced by that of the decay equation.

Considered with the same initial condition in (13), the equations (15) and (12) have exact solutions

$$\underline{u}(t) = \exp(-at)u^0, \tag{16}$$

and

$$u(t) = \frac{1}{b} W \left((b \exp(-at)u^0 \exp(bu^0)) \right), \tag{17}$$

respectively. The closed form expression (17) for the solution of the M-M equation is established in [11], on the basis of the Lambert W function, also called the Omega function or the product log, which is given by the relation

$$z = W(z) \exp(W(z)), \tag{18}$$

as the multivalued (single valued in the case when arguments are non negative real numbers) inverse of the non-injective complex-valued function

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

From the exact solutions in (16) and (17), we deduce the following intrinsic properties of the M-M equation:

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

$$0 \leq \underline{u}(t) \leq u(t) \leq u^0, \forall t \geq 0, \tag{19}$$

$$\lim_{b \to 0} u(t) = \underline{u}(t), \forall t \geq 0, \tag{20}$$

and

$$u(t) \downarrow 0 \ as \ t \to \infty, \tag{21}$$

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

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 $t = t_k$. Setting from (16) and (17), $\underline{u}^k = \underline{u}(t_k)$ and $u^k = u(t_k)$, the exact schemes of the decay and M-M equations are [6], [10]:

$$\underline{u}^{k+1} = \exp(-a\Delta t)\underline{u}^k \tag{22}$$

and

$$u^{k+1} = \frac{1}{b}W\left((b\exp(-a\Delta t)u^k \exp(bu^k))\right), \tag{23}$$

respectively. The exact scheme (22) is a non-standard finite difference (NSFD) scheme on observing that it is equivalent to

$$\frac{\underline{u}^{k+1} - \underline{u}^k}{\phi_1(\Delta t)} = -a\underline{u}^{k+1}, \tag{24}$$

or

$$\frac{\underline{u}^{k+1} - \underline{u}^k}{\phi_2(\Delta t)} = -a\underline{u}^k, \tag{25}$$

where

$$\phi_1(\Delta t) = \frac{\exp(a\Delta t) - 1}{a} \text{ and } \phi_2(\Delta t) = \frac{1 - \exp(-a\Delta t)}{a}. \tag{26}$$

In view of the property (20), that must be replicated by the numerical methods, the equivalent form [10]

$$\frac{u^{k+1} - u^k}{\phi_2(\Delta t)} = \frac{W\left((b\exp(-a\Delta t)u^k \exp(bu^k)) - bu^k\right)}{b\phi_2(\Delta t)}, \tag{27}$$

which is indeed a NSFD method, is useful for the exact scheme (23).

Despite the similarity in the dynamics of the M-M and decay equations, as stated in Theorem 1, the decay equation is not a good approximation of the M-M whenever the initial value u^0 is far away from the fixed-point $\tilde{u} = 0$. This fact which is in accordance with Hartman-Grobman theorem is illustrated in Figure 1 and Table 1 where the error $u^k - \underline{u}^k \geq 0$ is computed from the formulae (22) and (23). While the different rows display the expected convergence, the columns show the considerable discrepancy between u^k and $\underline{u}^k$ when the initial condition is far away from the fixed-point. Note that here and after, in the simulations involving the Lambert W function, we use the Matlab built-in function "lambertw(*)".

	$u^0 = 10$			$u^0 = 5.0$			$u^0 = 1.0$			$u^0 = 0.5$		
Δt	2	1	0.5	2	1	0.5	2	1	0.5	2	1	0.5
$\underline{u}^k$	1.35	1.35	1.35	0.68	0.68	0.68	0.14	0.14	0.14	0.07	0.07	0.07
u^k	8.20	8.20	8.20	3.39	3.39	3.39	0.28	0.28	0.28	0.10	0.10	0.10
$u^k - \underline{u}^k$	6.85	6.85	6.85	2.71	2.71	2.71	0.14	0.14	0.14	0.03	0.03	0.03

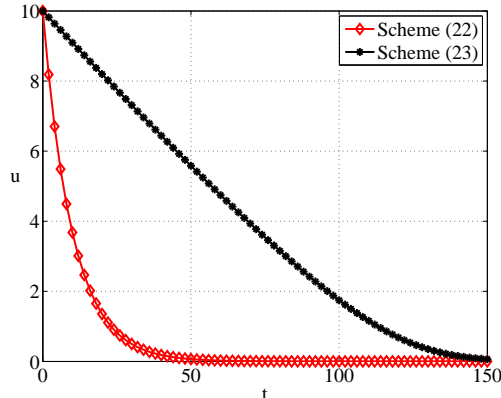Table 1: Error between solutions of M-M and decay equations for $a = 0.1$, $b = 1$ and $t = 20$.

Figure 1: Comparison of the exact schemes of M-M and decay equations for $u^0 = 10$ and $\Delta t = 2$.

3. Dynamically consistent NSFD schemes

Exact schemes that are effective in applications do not exist in many cases. This is specifically the case when the right-hand side of (12) has a more general form $f(u)$ including a term such as $-\dfrac{au^n}{1 + bu^n}$ that appears in the studies of chemostats, morphogenesis, continuous ventilation-volume, spruce budworm outbreak, calcium-stimulated-calcium release mechanism, etc. (see [10] and the references therein). In this section, we discuss briefly the following three NSFD schemes for the M-M equation, obtained in [9] by a judicious use of Mickens' rules [6] on the denominator of the discrete derivatives and the nonlocal approximation of nonlinear terms:

$$\frac{u^{k+1} - u^k}{\phi_1(\Delta t)} = -\frac{au^{k+1}}{1 + bu^k}, \tag{28}$$

$$\frac{u^{k+1} - u^k}{\phi_1(\Delta t)} = -\frac{au^{k+1}}{1 + bu^{k+1}}, \tag{29}$$

$$\frac{u^{k+1} - u^k}{\phi_2(\Delta t)} = -\frac{au^k}{1 + bu^k}. \tag{30}$$

While the schemes (28) and (30) are explicit, the implementation of the method (29) hinges on the fact that it is equivalent to a quadratic equation in u^{k+1}, with a unique nonnegative root given by

$$u^{k+1} = \begin{cases} \dfrac{bu^k - e^{a\Delta t} + \sqrt{(bu^k - e^{a\Delta t})^2 + 4bu^k}}{2b} & \text{if } b > 0, \\ u^k e^{a\Delta t} & \text{if } b = 0. \end{cases} \tag{31}$$

By analogy with the continuous model, we denote the sequence $\{u^k\}$ in (28)–(30) by $\{\underline{u}^k\}$ when $b = 0$. Thus, each $\underline{u}^k$ is a discrete solution of the decay equation (15). We have the following result that actually states more than the local property of elementary stability of all the NSFD schemes (28)–(30), which simply means that these schemes have only $\tilde{u} = 0$ as a fixed-point and this fixed-point is linearly stable as for the continuous model (see, e.g. [19] and [6]):

Theorem 2. *The NSFD schemes (28)–(30) 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*

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

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

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and

$$u^k \downarrow 0 \ as \ k \to \infty.$$

The message behind Theorem 2 is that the NSFD schemes (28), (29) and (30) perform as excellently as (23) or (27). This, along with the theory in Theorem 1, is supported by Figure 2 where $a = 0.1$, $\Delta t = 2$ while $b = 1$ and $b = 0$. In particular, for all the examples presented in this section, we take $a = 0.1$ and $\Delta t = 2$, which is considered to be large for standard numerical schemes.
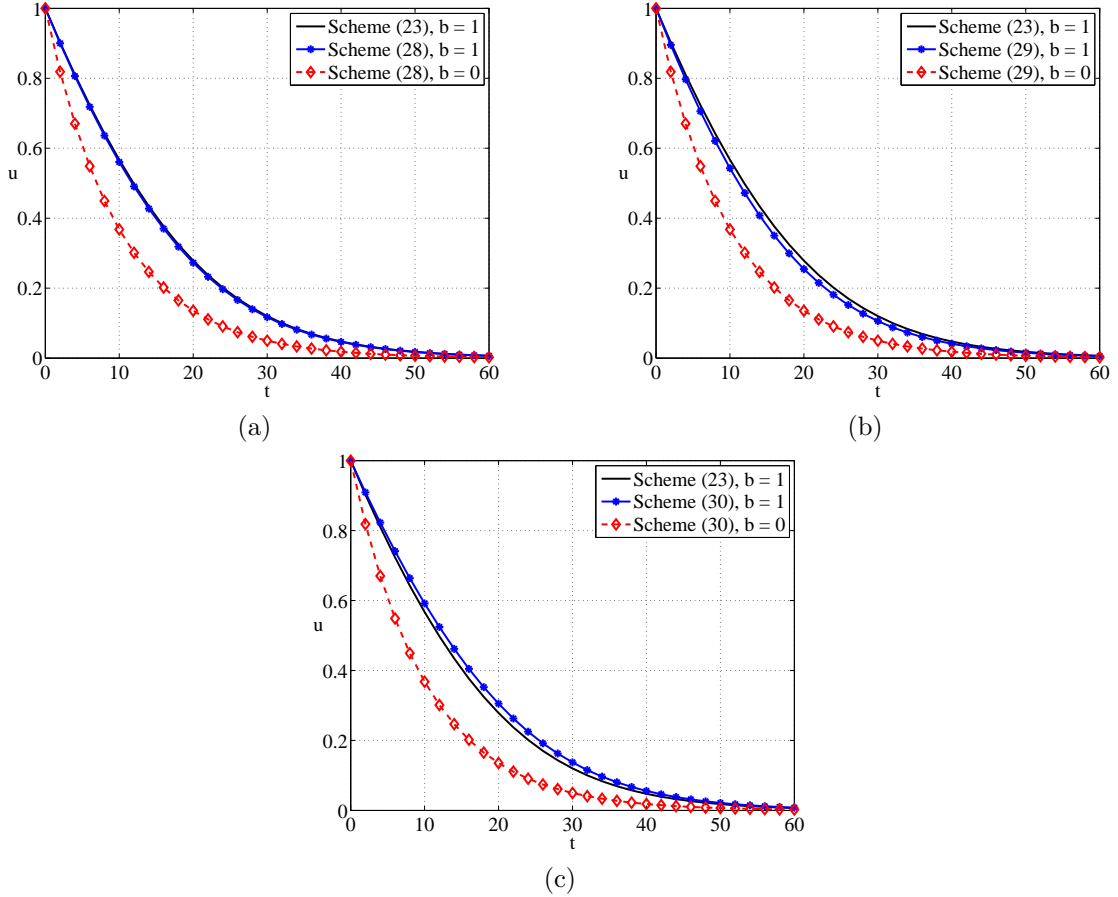

Figure 2: NSFD schemes (28), (29) and (30) versus the exact scheme (23).

On the contrary, the standard finite difference scheme

$$\frac{u^{k+1} - u^k}{\Delta t} = -\frac{au^k}{1 + bu^k}, \tag{32}$$

fails to have positive solutions, to satisfy all the above-mentioned properties for arbitrary values of Δt and to be elementary stable, as abundantly reported and illustrated in the literature (see, for instance, [19], [20], [6], [7] and [8]). Further comments on the power of the NSFD schemes presented in the paper are made in the concluding section.

In [9], the above study was extended to the advection and or diffusion equations with an M-M reaction term. The study of such partial differential equations is essential for the modeling of the spread in space of infectious diseases that are mentioned in the last section of this work. For simplicity, we consider the

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advection equation:

$$\frac{\partial u}{\partial t} + d\frac{\partial u}{\partial x} = -\frac{au}{1+bu}, \ d > 0, \ u(0,x) = u^0(x), \tag{33}$$

which under the condition $0 \le u^0(x) \le M$ admits a unique solution such that $0 \le u(t,x) \le M$. Since the solutions only move along the characteristics, which lead to the substitution $(t,x) \to U(t) := u(t, x+dt)$, the discrete analogue of which is $(k\Delta t, m\Delta x) \to u(k\Delta t, (m+k)\Delta x)$ whenever the functional relation

$$\phi_i(\Delta t) = \phi_i(d^{-1}\Delta x) \quad \text{i.e.,} \quad \Delta x = d\Delta t, \ i = 1, \ 2, \tag{34}$$

holds. We consider the following NSFD schemes for (33):

$$\frac{u_m^{k+1} - u_{m-1}^k}{\phi_1(\Delta t)} = -\frac{au_m^{k+1}}{1+bu_{m-1}^k}, \tag{35}$$

$$\frac{u_m^{k+1} - u_{m-1}^k}{\phi_2(\Delta t)} = -\frac{au_{m-1}^k}{1+bu_{m-1}^k}, \tag{36}$$

and

$$\frac{u_m^{k+1} - u_{m-1}^k}{\phi_2(\Delta t)} = \frac{W\left((b\exp(-a\Delta t)u_{m-1}^k\exp(bu_{m-1}^k)) - bu_{m-1}^k\right)}{b\phi_2(\Delta t)}. \tag{37}$$

All these NSFD schemes preserve the positivity and boundedness properties in the following precise manner:

Theorem 3. *Under the relation (34), we have*

$$0 \le u_m^0 \le M \Longrightarrow 0 \le u_m^k \le M, \forall k \ge 0, \forall m \in \mathbb{Z}, \ and \ \sup_m u_m^k =: S^k \downarrow 0 \ as \ k \to \infty.$$

Figure 3 illustrates the positivity and boundedness properties in Theorem 3 for the explicit NSFD scheme (35) with initial value $u^0(x) = e^{-x^2}$, $x \in \mathbb{R}$. Figure 3(a) shows a side-view profile corresponding to Figure 3(b) taken at $x = 0$. With $d = 0.1$ and $b = 1$, we take the space step size in accordance with (34), i.e. $\Delta x = 0.2$. The results compare nicely with the exact scheme-related method (37), as also shown in figure 4.
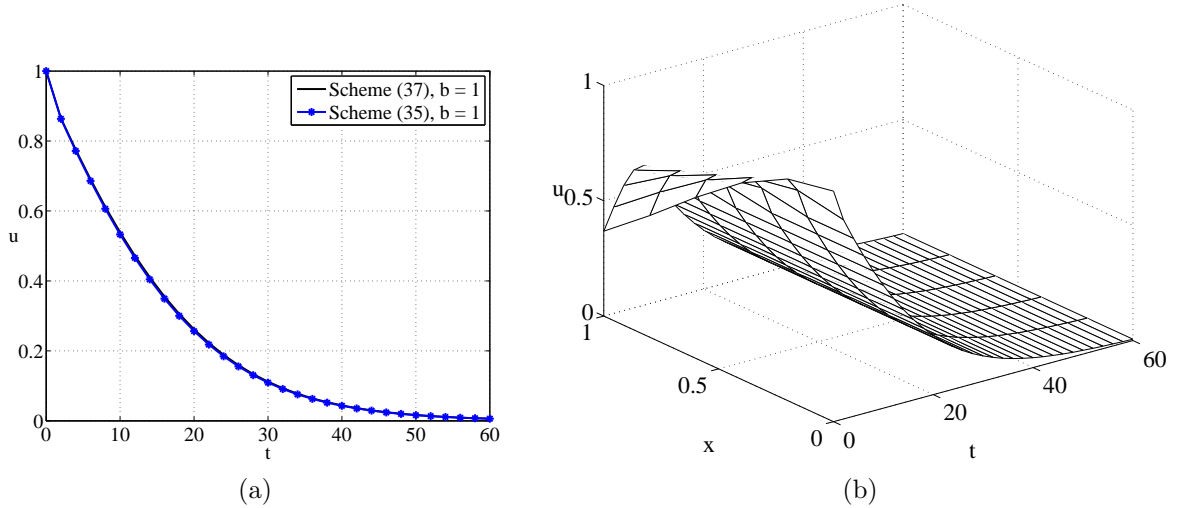

Figure 3: Positivity and boundedness of the NSFD scheme (35) versus the exact scheme-related method (37).
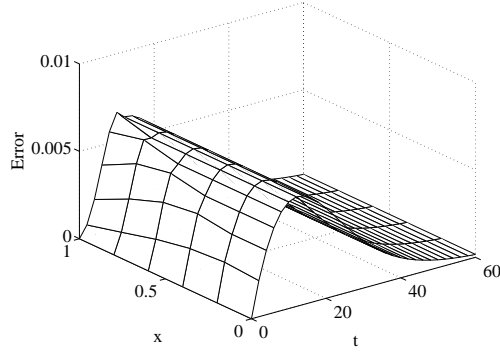
Figure 4: Error figure corresponding to Figure 3.

4. The SIR model

It is well-known that the mass action principle is not suitable for the modeling of the spread of diseases, specifically in the situation when the total population is very large. The standard incidence formulation is preferable [21]. More generally, one should assume that the number of adequate contacts per infective in unit time is a function of the total population in such a way that this number grows less rapidly as the total population increases [13], [14] and [17]. The Michaelis-Menten, as a functional response, captures well this fact and the tendency for the infective individuals to saturate. To be more specific, we assume that the total population N is divided into the three compartments consisting of susceptible (S), infectious (I) and recovered (R) individuals:

$$N = S + I + R.$$

The SIR model with M-M contact rate reads as

$$
\begin{aligned}
\frac{dS}{dt} &= \mu K - \frac{aSI}{1 + bI + bR + bS} - \mu S, \\
\frac{dI}{dt} &= \frac{aSI}{1 + bI + bR + bS} - (\mu + \gamma)I, \\
\frac{dR}{dt} &= \gamma I - \mu R,
\end{aligned}
\tag{38}
$$

where $K > 0$ is the carrying capacity, $\mu > 0$ is the natural death rate and $\gamma > 0$ is the recovery rate. By adding the equations in (38), we obtain the conservation law

$$\frac{dN}{dt} = \mu K - \mu N, \tag{39}$$

which has the exact scheme [6]

$$\frac{N_{k+1} - N_k}{\phi(\Delta t)} = \mu K - \mu N_{k+1} \text{ or } N_{k+1} = \frac{N_k + \mu\phi(\Delta t)K}{1 + \mu\phi(\Delta t)}, \tag{40}$$

where

$$\phi(\Delta t) = (1 - \exp(-\mu\Delta t))/\mu.$$

The dynamics of the SIR model is summarized in the following result [13], [14]:

Theorem 4.
(1) The system (38) is a dynamical system on the following biologically feasible compact set

$$\Omega = \{(S, I, R) \in \mathbb{R}_+^3; \ S + I + R \leq K\}.$$

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(2) The basic reproduction number and the disease-free equilibrium of the model are

$$\mathcal{R}_0 = \frac{aK}{(1+bK)(\mu+\gamma)} \ ,$$

and

$$E_* \equiv (S_*, I_*, R_*) = (K, 0, 0),$$

respectively.

(3) If $\mathcal{R}_0 \leq 1$, then E_* is globally asymptotically stable (GAS).

(4) If $\mathcal{R}_0 > 1$, then E_* is unstable. In this case, there exists a unique endemic equilibrium $E_\infty \equiv (S_\infty, I_\infty, R_\infty)$, which is locally asymptocally stable (LAS) and is given by

$$\begin{array}{rcl} S_\infty & = & K/\mathcal{R}_0, \\[4pt] I_\infty & = & \dfrac{\mu(1+bK)}{a}(\mathcal{R}_0 - 1), \\[4pt] R_\infty & = & K - S_\infty - I_\infty. \end{array}$$

We consider two types of NSFD schemes for the SIR model. The first type is motivated by Mickens' rules and the NSFD schemes (28)–(30) for the M-M. However, we present only the scheme related to (29) since it its implementation is not straightforward. The said NSFD scheme reads as follows:

$$\begin{array}{rcl} \dfrac{S_{k+1} - S_k}{\phi(\Delta t)} & = & \mu K - \dfrac{aS_{k+1}I_k}{1 + bI_k + bR_k + bS_{k+1}} - \mu S_{k+1}, \\[10pt] \dfrac{I_{k+1} - I_k}{\phi(\Delta t)} & = & \dfrac{aS_{k+1}I_k}{1 + bI_k + bR_k + bS_{k+1}} - (\mu+\gamma)I_{k+1}, \\[10pt] \dfrac{R_{k+1} - R_k}{\phi(\Delta t)} & = & \gamma I_{k+1} - \mu R_{k+1}. \end{array} \tag{41}$$

With

$$\begin{array}{rcl} A_k & = & b[1 + \mu\phi(\Delta t)], \\[4pt] B_k & = & (1 + bI_k + bR_k)[1 + \mu\phi(\Delta t)] - b[S_k + \mu K\phi(\Delta t)] + a\phi(\Delta t)I_k, \\[4pt] C_k & = & (1 + bI_k + bR_k)[S_k + \mu K\phi(\Delta t)], \end{array}$$

the implementation of (41) is done via the Gauss-Seidel structure:

$$\begin{array}{rcl} S_{k+1} & = & \dfrac{-B_k + \sqrt{(B_k)^2 + 4A_kC_k}}{2A_k}, \\[14pt] I_{k+1} & = & \dfrac{I_k + \phi(\Delta t)\dfrac{aS_{k+1}I_k}{1 + bI_k + bR_k + bS_{k+1}}}{1 + \phi(\Delta t)(\mu+\gamma)}, \\[14pt] R_{k+1} & = & \dfrac{R_k + \gamma\phi(\Delta t)I_{k+1}}{1 + \phi(\Delta t)\mu}. \end{array} \tag{42}$$

In order to motivate the second type of schemes, we focus on the equation

$$\frac{dS}{dt} = -\frac{aSI}{1 + bI + bR + bS}, \ \ S(0) = S_0. \tag{43}$$

For (43), we can in view of (23) or (27), consider the scheme

$$S_{k+1} = \frac{1 + bI_k + bR_k}{b\phi_k(\Delta t)} W\left[\frac{bS_k}{1 + bI_k + bR_k} \exp\left(\frac{bS_k}{1 + bI_k + bR_k} \right) \exp\left(\frac{-aI_k\Delta t}{1 + bI_k + bR_k} \right) \right],$$

or equivalently

$$\frac{S_{k+1} - S_k}{\phi_k(\Delta t)} = \frac{1 + bI_k + bR_k}{b\phi_k(\Delta t)} \times$$
$$\left\{ W\left[\frac{bS_k}{1 + bI_k + bR_k} \exp\left(\frac{bS_k}{1 + bI_k + bR_k} \right) \exp\left(\frac{-aI_k \Delta t}{1 + bI_k + bR_k} \right) \right] - \frac{bS_k}{1 + bI_k + bR_k} \right\}, \quad (44)$$

where

$$\phi_k(\Delta t) = \frac{1 + bI_k + bR_k}{aI_k} \left[1 - \exp\left(\frac{-aI_k \Delta t}{1 + bI_k + bR_k} \right) \right] = \Delta t + O[(\Delta t)^2] \quad (45)$$

for nonnegative I_k and R_k. For convenience, we put

$$S_{k,\Delta t} \; : \; = \frac{bS_k}{1 + bI_k + bR_k} \exp\left(\frac{bS_k}{1 + bI_k + bR_k} \right) \exp\left(\frac{-aI_k \Delta t}{1 + bI_k + bR_k} \right) \text{ and}$$

$$S_{k,0} \; : \; = \frac{bS_k}{1 + bI_k + bR_k} \exp\left(\frac{bS_k}{1 + bI_k + bR_k} \right) \quad (46)$$

from where we note, by definition (18) of the Lambert W function, that

$$W(S_{k,0}) = \frac{bS_k}{1 + bI_k + bR_k}. \quad (47)$$

Then, it is easy to check by the mean-value theorem and the differentiability property of the Lambert W function that we have the following approximation of the nonlinear term in (43):

$$(1 + bI_k + bR_k)\frac{W(S_{k,\Delta t}) - W(S_{k,0})}{b\phi_k(\Delta t)} = \frac{-aI_k S_k^*}{1 + bI_k + bR_k + bS_k^*} \approx \frac{-aI(t_k)S(t_k)}{1 + bI(t_k) + bR(t_k) + bS(t_k)}, \quad (48)$$

where

$$S_k^* = W\left[\frac{bS_k}{1 + bI_k + bR_k} \exp\left(\frac{bS_k}{1 + bI_k + bR_k} \right) \exp\left(\frac{-aI_k(\Delta t)\theta}{1 + bI_k + bR_k} \right) \right],$$

for some $\theta \in (0,1)$. At this stage, it is important to observe that

$$W(S_{k,0}) - W(S_{k,\Delta t}) \geq 0, \quad (49)$$

whenever S_k, I_k and R_k are nonnegative.

Based on the equations and notation in (44)–(48), we propose the following new NSFD scheme for the SIR model (38):

$$\frac{S_{k+1} - S_k}{\phi_k(\Delta t)} = \mu K + (1 + bI_k + bR_k)\frac{W(S_{k,\Delta t}) - W(S_{k,0})}{b\phi_k(\Delta t)} - \mu S_{k+1},$$

$$\frac{I_{k+1} - I_k}{\phi_k(\Delta t)} = -(1 + bI_k + bR_k)\frac{W(S_{k,\Delta t}) - W(S_{k,0})}{b\phi_k(\Delta t)} - (\mu + \gamma)I_{k+1},$$

$$\frac{R_{k+1} - R_k}{\phi_k(\Delta t)} = \gamma I_{k+1} - \mu R_{k+1}. \quad (50)$$

For the implementation of the NSFD scheme (50), we use its equivalent formulation:

$$S_{k+1} = \frac{1}{1 + \mu\phi_k(\Delta t)} \left[\mu K \phi_k(\Delta t) + \frac{1 + bI_k + bR_k}{b} W(S_{k,\Delta t}) \right],$$

$$I_{k+1} = \frac{1}{1 + (\mu + \gamma)\phi_k(\Delta t)} \left\{ I_k + \frac{1 + bI_k + bR_k}{b}[W(S_{k,0}) - W(S_{k,\Delta t})] \right\},$$

$$R_{k+1} = \frac{R_k + \gamma\phi_k(\Delta t)I_{k+1}}{1 + \mu\phi_k(\Delta t)}. \quad (51)$$

The NSFD scheme (50) differs from usual ones in that the denominator function varies with the discrete time, as seen from (45). However, this is not a problem in view of the asymptotic relation in (45) that, as mentioned earlier, holds due to the fact that the sequence $\dfrac{aI_k}{1 + bI_k + bR_k}$ is bounded for $I_k \geq 0$ and $R_k \geq 0$.

Theorem 5. *The NSFD schemes (41) and (50) are both dynamically consistent with the properties of the SIR model stated in Theorem 4 in the sense that we have the following facts:*
(1) The first scheme satisfies the discrete conservation law (40) and the second scheme satisfies a similar law with however the denominator function $\phi(\Delta t)$ replaced by $\phi_k(\Delta t)$ given in (45).
(2)
$$0 \leq S_0,\ I_0,\ R_0 \leq N_0 \leq K \Longrightarrow 0 \leq S_k,\ I_k,\ R_k \leq N_k \leq K.$$

(3) The NSFD schemes have no ghost fixed points. More so:
(3.1) If $\mathcal{R}_0 \leq 1$, then E_* is the only fixed point of the discrete system and this fixed-point is globally asymptotically stable;
(3.2) If $\mathcal{R}_0 > 1$, then E_* is unstable; E_∞ is the only additional fixed-point of the discrete scheme and this fixed-point is locally asymptotically stable.

Proof. The claim (1) is obvious by adding the respective equations in (41) and (50). Using this fact and the workable formulations (42) and (51) together with (49), the claim (2) follows. It is easy to check that the NSFD schemes have no ghost fixed points. Equally, it is easy to check the stability/instabilty of the fixed-points, which are hyperbolic, by linearization and by looking at the eigenvalues of the involved Jacobian matrices. Thus, what deserves some details is the global attractiveness of the disease-free fixed point which we outline below when $\mathcal{R}_0 < 1$. For the NSFD scheme (41), we have:

$$
\begin{aligned}
I_{k+1} &\leq \frac{1 + \phi(\Delta t)\dfrac{aS_{k+1}}{1 + bS_{k+1}}}{1 + \phi(\Delta t)(\mu + \gamma)} I_k \quad \text{from the second equation in (42)} \\
&= \frac{1 + \phi(\Delta t)\dfrac{1}{b}\dfrac{abS_{k+1}}{1 + bS_{k+1}}}{1 + \phi(\Delta t)(\mu + \gamma)} I_k \\
&\leq \frac{1 + \phi(\Delta t)\dfrac{aK}{1 + bK}}{1 + \phi(\Delta t)(\mu + \gamma)} I_k \quad \text{as the function } 0 \leq x \mapsto \frac{x}{1 + x} \text{ is increasing} \\
&= \frac{1 + \phi(\Delta t)\mathcal{R}_0(\mu + \gamma)}{1 + \phi(\Delta t)(\mu + \gamma)} I_k \quad \text{by definition of } \mathcal{R}_0 \text{ in Theorem 4.}
\end{aligned}
$$

When $\mathcal{R}_0 < 1$, we have
$$\frac{1 + \phi(\Delta t)\mathcal{R}_0(\mu + \gamma)}{1 + \phi(\Delta t)(\mu + \gamma)} < 1,$$
and the last estimate implies that
$$\lim_{k \to \infty} I_k = 0,$$
which if incorporated in the third and the first equations in (41) yields
$$\lim_{k \to \infty} R_k = 0 \text{ and } \lim_{k \to \infty} S_k = K.$$

This proves that the disease-free fixed-point E_* of the NSFD scheme (41) is globally attractive when $\mathcal{R}_0 < 1$. Regarding the global attractiveness of E_* for the scheme (50), the same procedure applies provided that in (51), we write the contribution of the Lambert W function with S_k^* as in the middle relation in (48). Then we replace S_{k+1} and $\phi(\Delta t)$ in the above reasoning with S_k^* and $\phi_k(\Delta t)$, respectively. $\qquad\square$

For numerical experiments, we take $a = 0.1$, $b = 1$, $K = 1000$ and $\Delta t = 2$ together with the following set of data:

μ	γ	$\mathcal{R}_0$	E_*	E_∞
0.2	0.1	0.333	$(1000, 0, 0)$	Not applicable
0.04	0.03	1.427	$(1000, 0, 0)$	$(700.77; 170.97; 128.33)$

Figures 5, 6, 7 and 8 illustrate Theorem 5 when the schemes (41) and (50) are used. The results are further displayed in Table 2. The performance of the exact related scheme (51) seems to be excellent when $\mathcal{R}_0 < 1$.

a. S.

b. I.
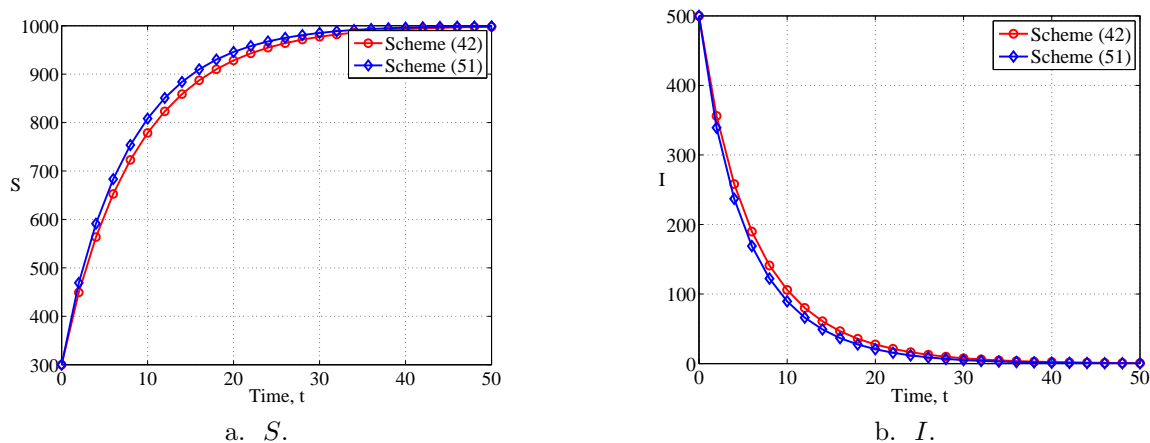
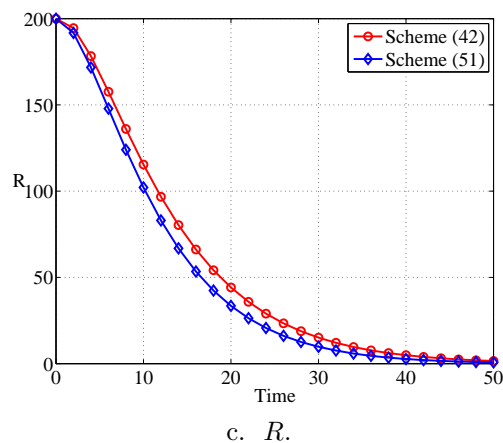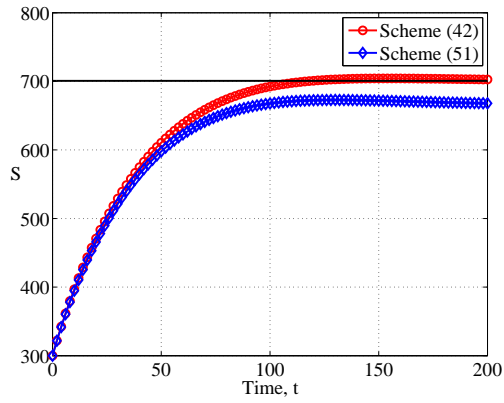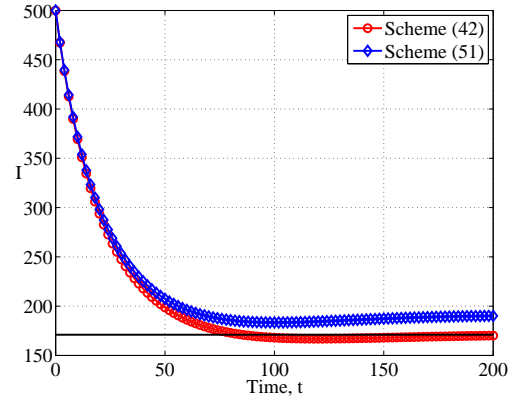Figure 5: Comparison of NSFD schemes (42) and (51) for $\mathcal{R}_0 < 1$.

c. R.

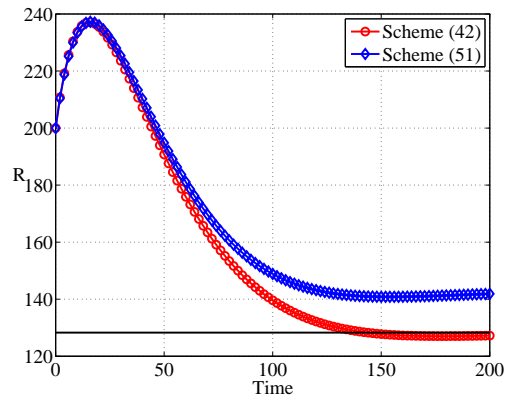Figure 6: Comparison of NSFD schemes (42) and (51) for $\mathcal{R}_0 < 1$.

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a. S.

b. I.

Figure 7: Comparison of NSFD schemes (42) and (51) for $\mathcal{R}_0 > 1$. The horizontal solid line denotes the endemic equilibrium solution.

c. R.

Figure 8: Comparison of NSFD schemes (42) and (51) for $\mathcal{R}_0 > 1$. The horizontal solid line denotes the endemic equilibrium solution.

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| | Solution I_k for $\mathcal{R}_0 > 1$ | | Solution I_k for $\mathcal{R}_0 < 1$ | |
$t = k\Delta t$	Scheme (42)	Scheme (51)	Scheme (42)	Scheme (51)
0	500	500	500	500
20	293.8048	298.1990	27.4599	20.6642
40	217.8604	225.2046	2.1706	1.2624
60	186.1466	196.2524	0.1785	0.0627
80	172.8557	185.7154	0.0147	0.0006
100	167.9855	183.3749	0.0012	0.0000
120	166.9604	184.3909	0.0001	0.0000
140	167.5036	186.3452	0.0000	0.0000
160	168.4890	188.1366	0.0000	0.0000
180	169.4146	189.4034	0.0000	0.0000
200	170.1108	190.1506	0.0000	0.0000

Table 2: Table of I_k solution for large k.

5. Conclusion

This paper is an extension of the authors' work [9] to the basic SIR epidemiological model where the contact between the susceptible individuals and the infected individuals is expressed by a nonlinear term which is similar to the right-hand side of the Michaelis-Menten ordinary differential equation. Using the specific form of the nonlinear term, we introduced new NSFD schemes based on the one hand on Mickens' rules [6] and on the other hand on the exact scheme of the M-M equation defined via the Lambert W function. We showed theoretically and computationally that the new NSFD schemes are dynamically consistent with the continuous model. The NSFD schemes that are not exact perform as efficiently as the exact-related schemes, confirming thus the power of the nonstandard approach. In addition, the designed schemes are very efficient compared to standard schemes. This is due mainly to the structure of the denominator function $\phi_i(\Delta t)$, which reflects the dynamics of the continuum models and which has very large permissible step size compared to standard schemes. In particular, all simulations were performed on an *Intel Core Quad CPU, 2.50GHz, 2.0GB RAM*, with a typical run requiring less than 2 seconds of computation time. The fact that the computer time is not a concern for NSFD schemes was also observed for complex and chaotic phenomena such as vibro-impact problems, see [22].

Our future interest is in the extension of the results of this study to more complex epidemiological models. In line with [23], a typical model we have in mind is the spread of diseases in space governed by the following advection-reaction-diffusion system:

$$\begin{aligned}
\frac{\partial S}{\partial t} + d\frac{\partial S}{\partial x} &= \mu K - \frac{aSI}{1 + bI + bR + bS} - \mu S + c\frac{\partial^2 S}{\partial x^2}, \\
\frac{\partial I}{\partial t} + d\frac{\partial I}{\partial x} &= \frac{aSI}{1 + bI + bR + bS} - (\mu + \gamma)I + c\frac{\partial^2 I}{\partial x^2}, \\
\frac{\partial R}{\partial t} + d\frac{\partial R}{\partial x} &= \gamma I - \mu R + c\frac{\partial^2 R}{\partial x^2}.
\end{aligned} \tag{52}$$

When there is no diffusion, $c = 0$, NSFD schemes can be obtained from the discrete advection schemes (35)-(37) combined with the approach in Section 4.

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