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Modelling And Simulation of Topical Drug Diffusion in The Dermal Layer of Human Body

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ABSTRACT

We consider the problem of drug diffusion in the dermal layer of human body. Two existing mathematical models of the drug diffusion problem are recalled. We obtain that the existing models lead to inconsistent equations for the steady state condition. We also obtain those solutions to the existing models are unrealistic for some cases of the unsteady state condition, because negative drug concentrations occur due to the inappropriate assumption of the model. Therefore, in this paper, we propose a modified mathematical model, so that the model is consistent, and the solution is nonnegative for both steady and unsteady state conditions of the drug diffusion problem in the dermal layer of human body. For the steady state condition, the exact solution to the proposed model is given. For unsteady state condition, we use a finite difference method for solving the models numerically, where the discretisation is centred in space and forward in time. Simulation results confirm that our proposed model and method preserve the non-negativity of the solution to the problem, so the solution is more realistic than that of the old model.

1. Introduction

There are several ways of medication. Some of them are by injection, pills, and topical medication. Each of them has its advantages and disadvantages. Medication by injection can make the drug directly follow the blood flow, but the injection needle causes pain. Medication by pills can make the drug follow the digestive system and follow the blood flow, but pills usually taste bitter, so they make inconvenient sensation. Topical medication may need more time for drug to be absorb in the human body. However, topical medication does not produce pain in general and it does not give bitter sensation, as the drug is placed on the surface of the skin.

A number of researchers reported their research results on topical drug diffusion problem in the dermal layer in human body [1-10]. Some of them use the molecular nanotechnology point of view [11-14]. In line with them, Sharma and Saxena [15] worked on finite element modelling in transdermal delivery system of drug especially when the case is at the steady state condition. Khanday and Rafiq [16,17] in a couple of papers reported their modelling and simulation modifying

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the model of Sharma and Saxena [15], so that the model is applicable for both steady and unsteady state conditions. However, we shall show that these existing mathematical models are unrealistic for some cases, because negative drug concentrations occur due to the inappropriate assumption of those models. Therefore, a new mathematical model preserving nonnegative drug concentration in the dermal layer should be proposed.

Our contributions in this paper are three folds. First, we show that the aforementioned existing models may produce unrealistic solution of the topical drug diffusion problem in the dermal layer in human body by showing that negative drug concentration may be produced by the existing model. Second, we propose a revised mathematical model for the topical drug diffusion problem in the dermal layer in human body, in which we consider one dermal layer of human body. Third, we provide finite difference numerical methods for solving these models, so that numerical simulations can be conducted.

The rest of this paper is arranged as follows. We begin with explaining the problem description of some existing models and the proposed resolution by revising the models, then we provide finite difference numerical scheme for solving the models. After that, results and discussion are presented. The paper is finally concluded with some remarks.

2. Methodology

In this section, two existing models of drug diffusion in the dermal layer are recalled. These existing models will be shown to have unrealistic solutions for some cases, as negative drug concentrations may be produced by the existing models. Therefore, we propose a modified model for the drug diffusion problem in the dermal layer. A sketch of one dermal layer of human body is shown in Figure 1, where the depth of the skin is from 0 to 1 unit of length. The drug is applied on the surface of the skin at space point $x = 0$. The drug diffuses downwards to points below the skin surface.

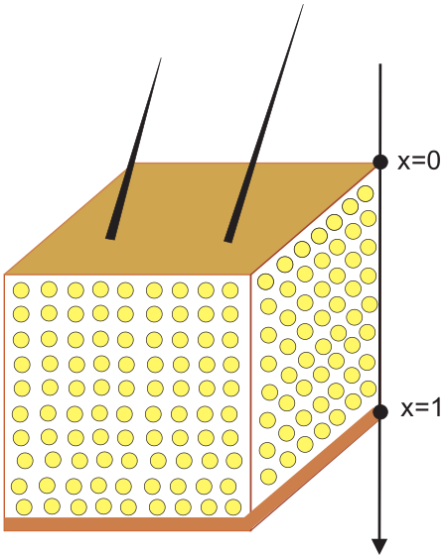

Fig. 1. A sketch of one dermal layer of human body where the depth x of the skin is from 0 to 1 unit of length. Here the skin materials on the considered space domain are assumed to be homogeneous with respect to the drug diffusion process

Some assumptions are taken as follows. In Figure 1, the surface of the skin is epidermis, where the thickness is up to about 0.1 mm. Below the epidermis is the dermis (dermal) layer, which is the domain of this paper. The dermal layer has the thickness of about 2 mm. As the domain of this research is the dermal layer, and we know that the epidermis is much thinner than the dermal layer, we assume that the position of the epidermis is at $x = 0$. Now, the thickness of 1 unit of length in Figure 1 can be obtained using scaling, that is, the depth positions of the original dermal layer are scaled by the maximum possible depth of the dermal layer. That is, 1 unit of length in Figure 1 is equivalent to 2 mm.

2.1 Existing Models and Their Weaknesses

Two existing mathematical models for describing drug diffusion in the dermal layer of human body are expressed in a general form

$$\frac{\partial u(x,t)}{\partial t} = \frac{\partial}{\partial x}\left(D\frac{\partial u(x,t)}{\partial x}\right) - A - B, \tag{1}$$

where x is the space variable, t is the time variable, $u(x,t)$ represents the drug concentration, D denotes the mass diffusivity, A represents the rate of drug absorption by the tissue, and B is the rate of drug intake by the blood. Similar forms to Eq. (1) were given previously by Crank [18] for some diffusion problems. Eq. (1) was used by Sharma and Saxena [15] for the case of the steady state condition of drug diffusion in the dermal layer of human body, where A and B are assumed to be positive constants.

In addition, Eq. (1) was used by Khanday and Rafiq [16,17] for the cases of steady and unsteady state conditions of drug diffusion in the dermal layer of human body. Khanday and Rafiq [16,17] assumed that A is based on the law of mass action, that is, the rate of drug absorption by the tissue is a decreasing function with respect to the drug concentration, so is assumed to be

$$A = \exp(-ku), \tag{2}$$

where for one dermal layer, k is assumed to be a positive constant. Sharma and Saxena [15] as well as Khanday and Rafiq [16,17] took D to be a positive constant.

Let us analyse Eq. (1). Physically, the value of D is dependent on , x, and t, but taking D a positive constant is still reasonable, as the layer of dermal region is very thin and one layer can be regarded as a uniform homogeneous material. However, taking A and B positive constants is unrealistic; because if we have zero concentration of drug, then Eq. (1) is inconsistent, as it becomes

$$0 = -A - B. \tag{3}$$

Furthermore, taking A as defined in Eq. (2) is still unrealistic because of a similar reason; that is, when we have $u(x,t) = 0$, then Eq. (1) becomes

$$0 = -1 - B, \tag{4}$$

which is an inconsistent equation, as B is defined to be nonnegative.

In the next subsection, we write our proposed model to overcome these inconsistent equations due to the inappropriate assumption in the existing models.

2.2 Proposed Model

Recall that A represents the rate of drug absorption by the tissue, and B is the rate of drug intake by the blood. The terms A and B should be dependent on the drug concentration $u(x,t)$, instead of constants. We assume that

$$A = k_1 u(x,t), \tag{5}$$

where k_1 is a positive constant. Eq. (5) means that the value of A is proportional with the drug concentration. In addition, we assume that

$$B = k_2 u(x,t), \tag{6}$$

where k_2 is a positive constant. That is, the value of B is also proportional with the drug concentration.

Therefore, our proposed model for drug diffusion in the dermal layer of human body is

$$\frac{\partial u(x,t)}{\partial t} = D\frac{\partial^2 u(x,t)}{\partial x^2} - k_1 u(x,t) - k_2 u(x,t), \tag{7}$$

where k_1 and k_2 are positive constants and the mass diffusivity D is assumed to be constant. For the steady state condition, model (7) becomes

$$0 = D\frac{d^2 u(x)}{dx^2} - Ku(x), \tag{8}$$

where $K = k_1 + k_2$.

Suppose that we consider the drug diffusion problem with the space domain $[0,1]$, as illustrated in Figure 1, where the boundary conditions are

$$u(0,t) = \alpha, \tag{9}$$

and

$$u(1,t) = \beta, \tag{10}$$

in which α and β are nonnegative constants. For the steady state condition, the exact solution to the proposed model (7) can be obtained by solving Eq. (8). The exact solution to model (7) for the steady state condition is

$$u(x,t) = c_1 \exp(mx) + c_2 \exp(-mx), \tag{11}$$

where

$$m = \sqrt{K/D}, \tag{12}$$

and

$$c_1 = \frac{\alpha \exp(-m) - \beta}{\exp(-m) - \exp(m)}, \tag{13}$$

as well as

$$c_2 = \frac{\alpha \exp(m) - \beta}{\exp(m) - \exp(-m)}. \tag{14}$$

For the unsteady state condition, it is easier for us to implement numerical methods for solving both the existing equation model (1) and the proposed equation model (7), as we provide in the next subsection.

2.3 Numerical Methods

This subsection is devoted to numerical methods for solving the existing and proposed models. We implement finite difference methods, where discretisation is forward in time and centred in space. Suppose that the space domain is $[0, L]$ and the time domain is $[0, T]$, where L represents the depth of the skin (dermal region) of interest, and T is the final time of the simulation. The space domain $[0, L]$ is discretised into a finite set of points $\{x_0 = 0, x_1, x_2, x_3, \ldots, x_m = L\}$, where $\Delta x = x_i - x_{i-1}$ for $i = 1, 2, 3, \ldots, m$. The time domain $[0, T]$ is also discretised into a finite set of points $\{t^0 = 0, t^1, t^2, t^3, \ldots, t^n = L\}$, where $\Delta t = t^j - t^{j-1}$ for $j = 1, 2, 3, \ldots, n$. Here, $x_i = i\Delta x$ for $i = 0, 1, 2, \ldots, m$ and $t^j = j\Delta t$ for $j = 0, 1, 2, \ldots, n$. We denote $u_i^j \approx u(x_i, t^j)$.

2.3.1 A finite difference method for the existing model

Using finite differences for derivatives, Eq. (1) can be discretised as

$$\frac{u_i^{j+1} - u_i^j}{\Delta t} = D \frac{u_{i+1}^j - 2u_i^j + u_{i-1}^j}{(\Delta x)^2} - (A + B). \tag{15}$$

Rewriting (15), we obtain the finite difference scheme for solving Eq. (1) as follows

$$u_i^{j+1} = u_i^j + \frac{D\,\Delta t}{(\Delta x)^2}\left(u_{i+1}^j - 2u_i^j + u_{i-1}^j\right) - C\,\Delta t, \tag{16}$$

where $C = A + B$. For zero concentration of drug everywhere, finite difference scheme (16) matches with the inconsistent Eq. (3).

2.3.2 A finite difference method for the proposed model

Similar to the previous discretisation of Eq. (1), we discretise Eq. (7) using finite differences for derivatives, so we have

$$\frac{u_i^{j+1} - u_i^j}{\Delta t} = D \frac{u_{i+1}^j - 2u_i^j + u_{i-1}^j}{(\Delta x)^2} - k_1 u_i^j - k_2 u_i^j. \tag{17}$$

Rewriting (17), we obtain the finite difference scheme for solving Eq. (7) as follows

$$u_i^{j+1} = u_i^j + \frac{D\,\Delta t}{(\Delta x)^2}\left(u_{i+1}^j - 2u_i^j + u_{i-1}^j\right) - K\,\Delta t\,u_i^j, \tag{18}$$

where $K = k_1 + k_2$. We observe that finite difference scheme (18) leads to a consistent equation when we have zero drug concentration everywhere.

As our numerical methods are explicit, in the numerical implementations, the value of time step Δt must be taken not too large by considering the value of space step Δx. This is so as to stabilise the finite difference methods.

3. Results and Discussion

In our simulations, quantities are dimensionless, where their corresponding dimensional units are as follows: length is measured in micrometers $(\mu\mathrm{m})$; time in seconds (s); mass in miligrams (mg); concentration in miligrams per meter $(\mathrm{mg\,m^{-1}})$; A and B in $\mu\mathrm{m}^{-1}$; and D in $\mu\mathrm{m}^2\mathrm{s}^{-1}$. With these conventions, we shall not write the units for simplicity of writings. We take $L = 1$ and T can be taken based on the time of interest. The boundary conditions are

$$u(0,t) = 5, \tag{19}$$

and

$$u(1,t) = 0. \tag{20}$$

3.1 Results and Discussion for the Existing Models

We provide two test cases of the existing models. The first is based on the work of Sharma and Saxena [15]. The second is based on the work of Khanday and Rafiq [16,17].

For the first test, we consider Eq. (1) where $A = 0.0001$, $B = 0.002$, and $D = 0.00068$, as taken by Sharma and Saxena [15]. In the finite difference method, we take $\Delta x = 0.01$ and $\Delta t = 0.5\Delta x$. The results of this simulation are shown in Figure 2 and Figure 3. Figure 2 seems to show realistic results. However, we observe that Figure 3 (which is a magnification of Figure 2 around the x-axis) contains negative concentration in the dermal layer, which is unrealistic. The drug concentration is nonnegative everywhere in reality.

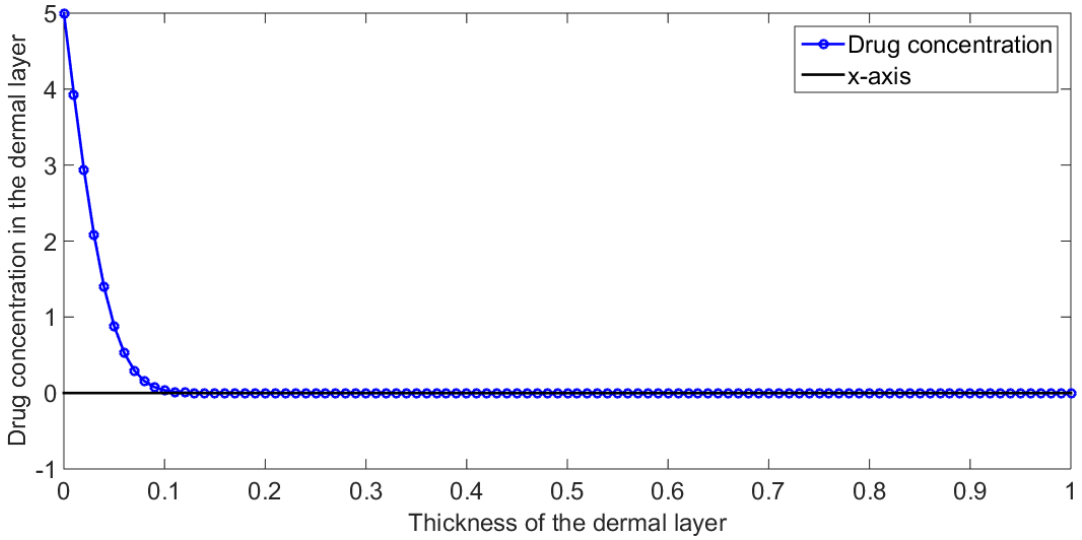

Fig. 2. Simulation results of the model of Sharma and Saxena [15] at time $t = 1$. These results seem to be realistic, but in fact, unrealistic when they are magnified as in Figure 3, because it contains negative drug concentrations

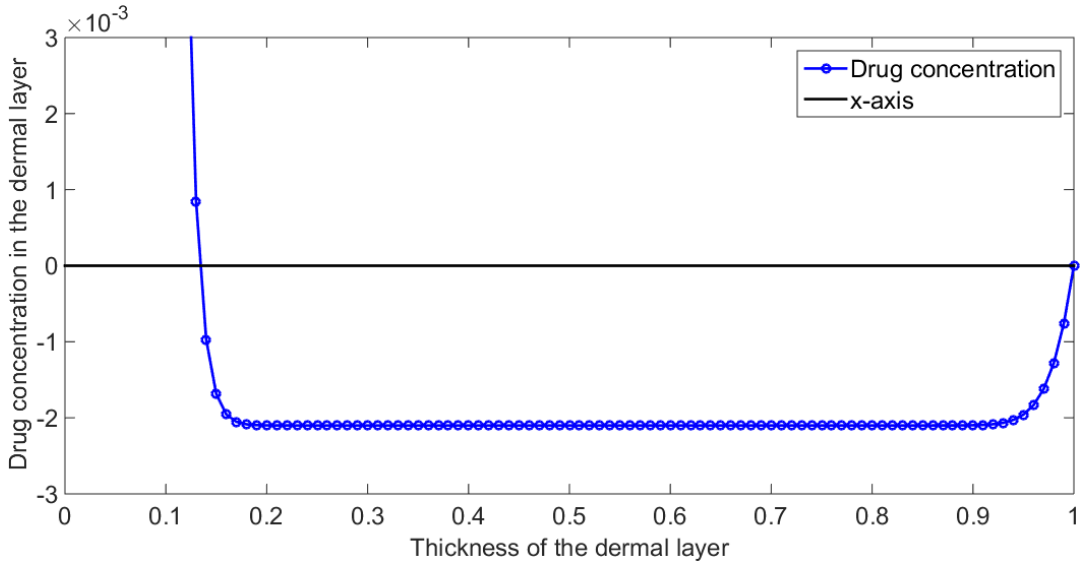

Fig. 3. A magnification of Figure 2 around the x-axis at time $t = 1$. These results are unrealistic, because of the negative drug concentration occurrence

For the second test, we consider Eq. (1), where $k = 0.4$, $B = 0.002$, and $D = 0.00068$, as taken by Khanday and Rafiq [16,17]. In the finite difference method, again, we take $\Delta x = 0.01$ and $\Delta t = 0.5\Delta x$. The results of this simulation are shown in Figure 4. We observe without any magnification that Figure 4 contains negative concentration, which is also unrealistic.

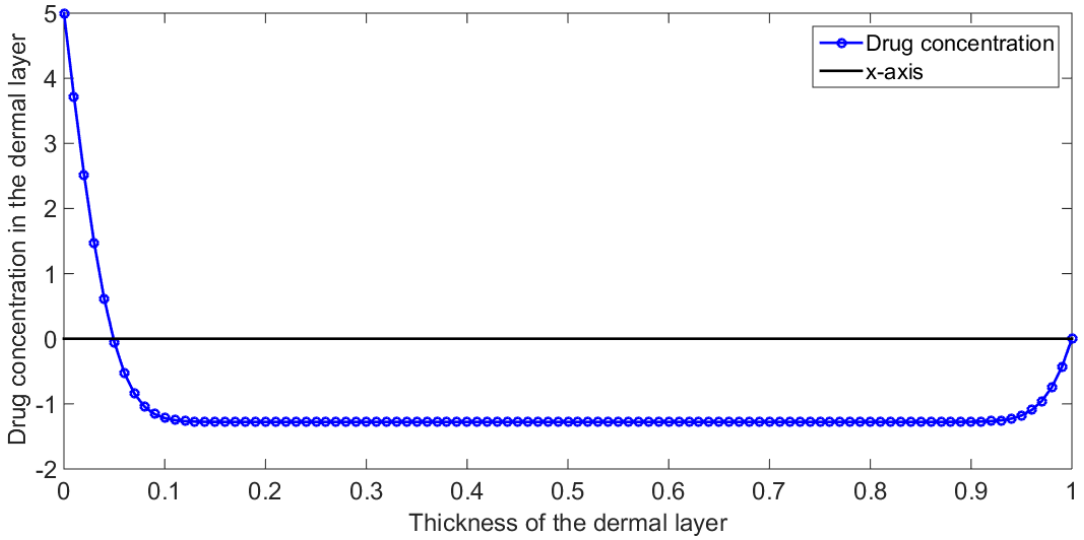

Fig. 4. Simulation results of the model of Khanday and Rafiq [16,17] at time $t = 1$. These results are unrealistic due to the negative drug concentration occurrence

3.2 Results and Discussion for the Proposed Model

In this test, we consider Eq. (7) where $k_1 = 0.02$, $k_2 = 0.002$, $D = 0.00068$. In the finite difference method, again, we take $\Delta x = 0.01$, but $\Delta t = 5\Delta x$, so that the computation is faster.

The results of this simulation are shown in Figure 5 illustrating the computational results at time $t = 1, 3600, 36000$. There is no negative concentration in this figure, even when we magnify Figure 5 to be Figure 6, we do not observe negative concentration. In this test, we consider the solution at time $t = 1$, that is, 1 second after the drug is applied on the skin; we obtain that the solution is more realistic than those of existing models, as the solution is a decreasing function, and no negative value of the solution occurs.

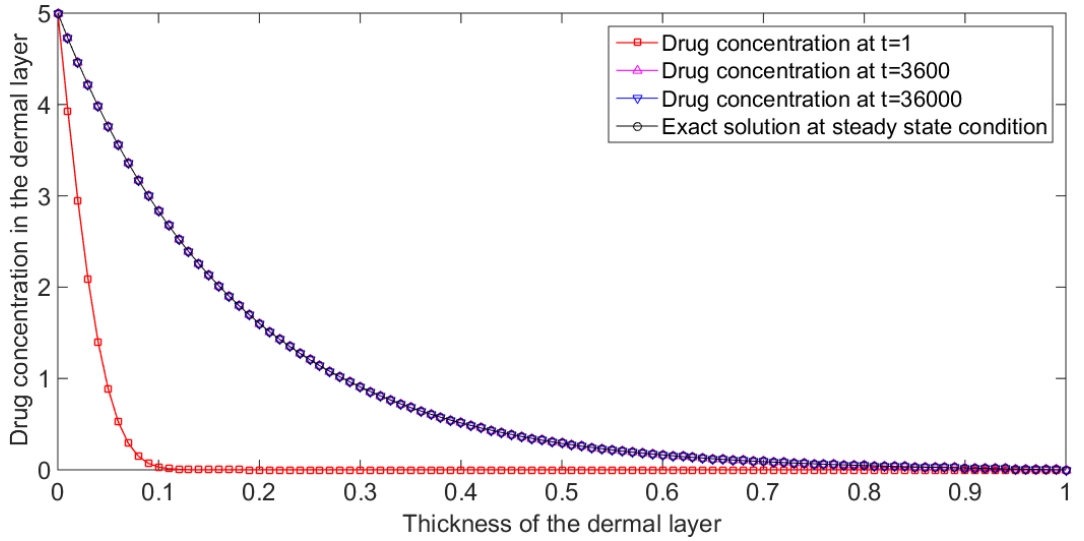

Fig. 5. Simulation results of the proposed method at time $t = 1, 3600, 36000$. These are realistic, as the solution is a decreasing function, and no negative value of the solution occurs

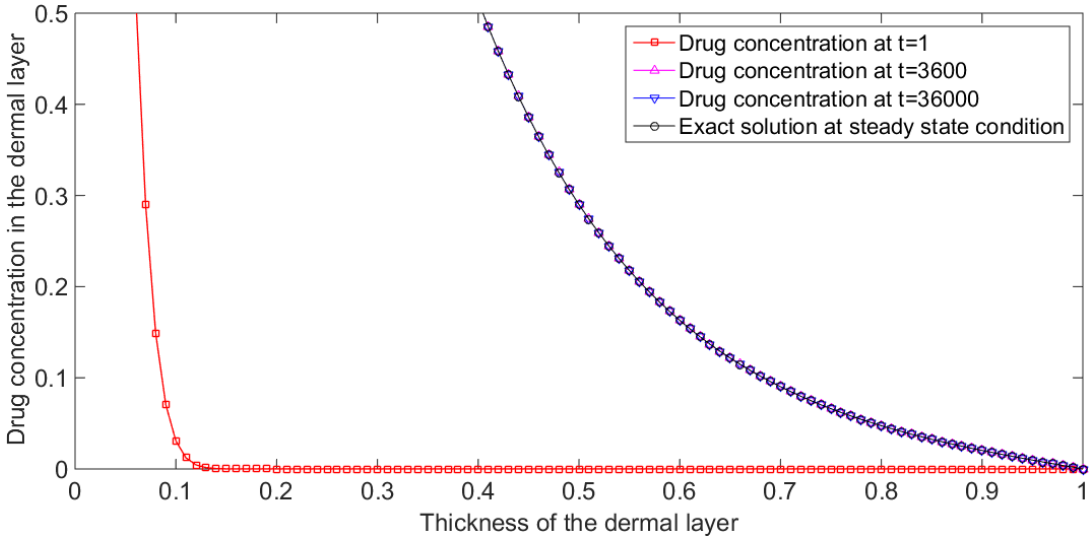

Fig. 6. A magnification of Figure 5 around the x-axis at time $t = 1, 3600, 36000$. These are realistic, as the solution is a decreasing function, and no negative value of the solution occurs

After 1 hour (3600 seconds), the solution has achieved the steady state condition. This steady state condition is confirmed with the fact that even when we continue the simulation until, say, 10 hours (36000 seconds) the solution does not change. We obtain that the solution at time $t = 3600$ coincides with the solution at a later time, such as at time $t = 36000$. In fact, both finite difference solutions at $t = 3600$ and $t = 36000$ coincide with the exact solution (11) up to the machine precision. All of these solutions are realistic, as they are decreasing with respect to the dermal depth x connecting the concentration value at the surface $x = 0$ and the concentration value at the deepest point $x = 1$, and there is no negative concentration occurrence on the spatial-temporal domain.

With the success of our strategies involved in the proposed model and method, we believe that these results could be extended further in other fluid mechanics and heat transfer areas as well as initial-boundary value problems. One could implement our strategies to various problems (to mention some of them, see Alawi and Kamar [19], Bindu *et al.,* [20], Ewis [21], Ferdows *et al.,* [22], Ghani and Jami [23], Giap and Kosuke [24], Jamil *et al.,* [25], Mohamed *et al.,* [26], Sahak *et al.,* [27] and the work of Mungkasi [28,29] as well as Mungkasi and Roberts [30]). Each of these problems could be explored and solved in their own rights.

4. Conclusions

We have achieved three objectives of this paper. First, we have shown that two existing mathematical models of drug diffusion in the dermal layer of human body produce unrealistic solution for some cases due to the negative drug concentration occurrence. Second, we have proposed a revised mathematical model for drug diffusion in the dermal layer of human body. Third, we provide finite difference schemes for solving the mathematical models. We obtain that our proposed mathematical model solved using the finite difference method produces a more realistic solution for drug diffusion problem in the dermal layer of human body. Further research direction could incorporate laboratory experiments to obtain accurate parameter values regarding our proposed model.

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