

## Article

# Axial Diffusion of the Higher Order Scheme on the Numerical Simulation of Non-steady Partial Differential Equation in the Human Pulmonary Capillaries

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**Abstract:** In the present study, a mathematical model of non-steady partial differential equation from the process of oxygen mass transport in the human pulmonary circulation is proposed. Mathematical modelling of this kind of problems lead to a non-steady partial differential equation and for its numerical simulation, we have used finite differences. The aim of the process is the exact numerical analysis of the study, wherein consistency, stability and convergence is proposed. The necessity of doing the process is that, we would like to increase the order of numerical solution to a higher order scheme. An increment in the order of numerical solution makes the numerical simulation more accurate, also makes the numerical simulation being more complicated. In addition, the process of numerical analysis of the study in this order of solution needs more research work.

**Keywords:** non-steady partial differential equation; higher order finite difference scheme; axial diffusion; convergence; consistency; stability

**MSC:** Primary: 35-02, 35B30, 35B35, 35B65. Secondary: 92B05

## 1. Introduction

A brief review literature is given as follows: Wu et al. [1] have presented a numerical simulation of blood flow in two anarysmal vessels, using mixture theory, the velocity fields and spatial distribution of the red blood cell-induced platelet transport in Saccular Aneurysms and the plasma are predicted. Bridges et al. [2] have studied the flow of a shear-thinning, chemically-reacting fluid that could be used to model the flow of the synovial fluid. They have solved the balance of linear momentum together with a convection-diffusion equation. Hund and Antaki [3] have proposed an extended convection-diffusion model based on the diffusive balance of a fictitious field potential, that accounts for the gradients of both the dilute phase and the local hematocrit. Wu and Massoudi [4] have studied the effects of dissipation in the couette flow and heat transfer in a drilling fluid, and explore the effects of concentration and the shear-rate and temperature-dependent viscosity, along with a variable thermal conductivity. Massoudi and Antaki [5] have developed a model for blood using the theory of interacting continua, that is, the mixture theory. They have discussed, a framework for modelling the rheological behavior of blood. Skorczewski et al. [6] have considered computational simulations using a 2D lattice-Boltzmann immersed boundary method were conducted to investigate the motion of platelets near a vessel wall and close to an intravascular thrombus. Burger's equation [7] (Johannes Martinus Burger), a Dutch scientist, devised a simplified form of Navier-Stokes equation, in the presence of convective term and diffusive term wherein uses the study of opposite effects of convection and diffusion at a basic level.

This equation is fundamental in modelling shockes and has found immense application in area of viscous flow, such as blood flow in a creeping fluid. Zhan and Wang [8] have studied mathematical modelling of convection enhanced delivery (CED) of chemo-therapeutic drugs which can successfully bypass the blood-brain barrier. The modelling demonstrates the advantages of convection enhanced delivery in enhancing the convective flow of intenstitial fluid and reducing the drug concentration dilution caused by the fluid loss from blood stream in the tumour region around the infusion site. The delivery outcomes of the drug in CED treatments are strongly dependent on its physico-chemical properties. Kaesler et al. [9] computed computational modelling of oxygen transfer in artificial lungs. Their study introduces an approach to model the oxygen transfer in blood on a fiber level with CFD. Plasma and RBCs were implemented as two phases and the reaction of hemoglobin and oxygen to oxyhemoglobin was included in the convection-diffision equation in form of a source term. Melnik and Jenkins [10] concentrated on computational control of flow in airblast atomisers for pulmonary drug delivery. In the paper, PDD systems based on airblast atomisation have been analysed mathematically. Mountrakis et al. [11] simulated RBCs and platelets to explore their transport behavior in aneurysmal geometries. They considered two aneurysms with different aspect ratios in presence of fast and slow blood flows, and examined the distributions of the cells. Whittle et al. [12] suggest that the presence of intra-aneurysmal clot in giant intracranial aneurysms has little prognostic significance and does not alter the management or outcome after treatment. Hirabayashi et al. [13] considered a lattice Boltzmann simulation of blood flow in a vessel deformed by the presence of an aneurysm. They propose a stent positioning factor as characterizing tool for stent pore design in order to describe the flow reduction effect and reveal the several flow reduction mechanisms using this effect. Weir [14] is reviewed the pathological, radiological, and clinical information regarding unruptured intracranial aneurysm. The author concluded that the current state of knowledge about unruptured aneurysms does not support the use. The largest diameter of the lesion as the sole criterim on which to base treatment decisions, although it is undoubted importance.

Now, apart from the above discussion on convective-diffusion equations and in the remaining short span of the time and pages in this study, we try to examine higher order finite difference scheme to approximate time-dependent partial differential equation including axial and radial diffusions with convective effect of the blood. The standard convection-diffusion model is based on continuum approach wherein we are using here. Also, our approach want to examine the effect of axial diffusion since normally most of the models consider only radial diffusion as we did in our previous studies. Here, it should be mentioned that, to our knowledge this happens for the first time in this order of magnitude. Further, this kind of equation has application in bio-engineering problems, e.g., propagation of material [15], boundary layer of fluids, electrical circuits in cables and the mass transfer problems with respect to the conditions [16–26]. In addition, our discussion is on the convergence, consistency, and stability [27] of finite differences equations which describe the model.

## 2. Mathematical Description of the Model as a Whole

Let us consider at first, the RBC distribution and the blood flow transport. When we have succeeded, we can add aneurysms wherein it has been described in the different literature in introduction in our future study.

In the pulmonary capillaries, we have:

$$\frac{\partial c_i(p, t)}{\partial t} = -\nabla \cdot J_i(p, t) + R_i(p, t), \quad (1)$$

where  $c_i(p, t)$  is the concentration of the  $i$ -th species (i.e., oxygen or carbondioxide) at the position  $p$  and the time  $t$ . Position  $p$  in Cartesian co-ordinate is  $(x, y, \zeta)$  or in polar co-ordinate is  $(r, \theta, \zeta)$  with an origin [22]. The quantity  $J_i(p, t)$  is equivalent to the sum of the fluxes of species and  $R_i(p, t)$  is the reaction due to non-linearity of the  $i$ -th species in a unit quantity. Flux vector is the sum of two vectors

of convection and diffusion and is according the Fick's first law of diffusion. Hence, the mass balance in the Equation (1) for the  $i$ -th species is[24]:

$$\frac{\partial c_i(p, t)}{\partial t} = -\nabla \cdot [v(p, t)c_i(p, t) - D_i(p)\nabla c_i(p, t)] + R_i(p, t), \quad (2)$$

even due Equation (2) is in capillaries, it can be written more precisely as:

$$\frac{\partial c_i(x, r, t)}{\partial t} = -v(r)\frac{\partial c_i(x, r, t)}{\partial x} + D_i\nabla^2 c_i(x, r, t) + R_i(x, r, t), \quad (3)$$

71 where  $\nabla^2 = \frac{\partial^2}{\partial r^2} + r^{-1}\frac{\partial}{\partial r} + \frac{\partial^2}{\partial x^2}$ .

72 Initial condition  $c_i(x, r, 0)$  can be taken arbitrary, or with the solution of the steady-state  
73 Equation (3) as a whole. Boundary conditions could be as the following:

74 (i) concentration in the beginning is zero or finite and for the flux (radial)  $\frac{\partial c_i(x, r, t)}{\partial x}$  at  $x = L$  (at the end  
75 of capillary) is constant,

76 (ii)  $\frac{\partial c_i(x, 0, t)}{\partial r} = 0$  (symmetry at the center of capillary), and

77 (iii) another condition is at the capillary wall where the derivative of the equations will be considered,  
78 wherein depend on the species. For oxygen which is combined with the hemoglobin inside RBCs,  
79 concentration in Equation (3) is the concentrations of plasma and RBCs. Hence, the diffusion has two  
80 components, first diffusion in plasma and the second, diffusion of oxygen which is corresponded to  
81 the diffusion of oxygen in the RBCs.

## 82 2.1. In the Tissues

We have the following:

$$\frac{\partial c_i(p, t)}{\partial t} = \nabla \cdot [D_i(p)\nabla c_i(p, t)] + R_i(p, t), \quad (4)$$

hence, in tissue and at polar co-ordinate, we have:

$$\frac{\partial c(x, r, t)}{\partial t} = D\nabla^2 c(x, r, t) + R(t). \quad (5)$$

## 83 2.2. Transport Inside the Components

Differential equations is inside the tissues, and if we want the space of the cells, we should add again boundary conditions. A condition in connection of blood concentration and tissue condition which is regarding the influence of capillary wall. With continuity assumption of the capillary wall, we have:

$$c(x, a, t)|_b = \frac{c(x, a, t)}{\alpha}|_t, \quad (6)$$

$$D\frac{\partial c(x, a, t)}{\partial r}|_b = D\frac{\partial c(x, a, t)}{\partial r}|_t, \quad (7)$$

where  $b$  and  $t$  stands for blood and tissue. Equation (6) announce that blood in the capillary wall is equivalent to that of tissue (with a coefficient of  $\alpha$ ) and Equation (7) expresses that there is a balance between capillary and the tissue. If the capillary wall has a permeability, the Equations (6) and (7) will be:

$$\begin{aligned} -[D\frac{\partial c(x, a, t)}{\partial r}]|_b &= p(x)[c_b(x, a, t) - \frac{c_t(x, a, t)}{\alpha}] = \\ &= -[D\frac{\partial c(x, a, t)}{\partial r}]|_t. \end{aligned} \quad (8)$$

At the end, mathematical models for the description of transport equations in the pulmonary capillary and surrounding tissue is considered in this section. Equations (1)–(7) show the vector flux of the convection and diffusion which is based on Fick's first law of diffusion. These equations are described in Cartesian and polar co-ordinates. For solution of equation, arbitrary initial condition and boundary conditions of (i) to (iii) is required. If capillary wall has a permeability, Equation (8) can be used [29].

### 3. Mathematical Description of the Model in the Present Study

New, we consider the following time-dependent partial differential equation as a simplification of section 2. Such an equation occurs in the transport of oxygen in a slab of capillary which depends on the unsteady transport by convection and the unsteady diffusion (axial as well as radial in the directions). The capillary is assumed to be a 2D channel of thickness  $2a$  and  $a = 1$ , respectively. Hence, the equation is:

$$c_t + uc_y = D(c_{xx} + c_{yy}), \quad (9)$$

for  $0 \leq x \leq 1$ ;  $0 \leq y \leq 1$  and  $t > 0$ . In the capillary slab, the flow is laminar and is assumed to be uniform with an average velocity  $u = 0.4$ , and the diffusion coefficient of oxygen is considered as a constant quantity,  $D = 0.24$ . The first and second terms on the left-side are respectively the rate of change of concentration per unit time and the transport due to convection whereas the terms on the right-side indicate the free molecular diffusion in the radial as well as axial directions. Equation (9) is to be solved under the following boundary, entrance and initial conditions.

(i) Boundary conditions:

(a) the flux of flow during the line of symmetry is zero, e.g.,

$$c_x(0, y, t) = 0; \text{ for } \forall t \text{ and } 0 \leq y \leq 1, \quad (9a)$$

(b) at the wall of horizontal line, we have:

$$c(1, y, t) = 1; \text{ for } \forall t \text{ and } 0 \leq y \leq 1, \quad (9b)$$

(ii) Entrance conditions:

(c) in the start of axial direction, we have:

$$c(x, 0, t) = 0; \text{ for } \forall t \text{ and } 0 \leq x \leq 1, \quad (9c)$$

(d) and at the wall of axial direction for the flux, we have:

$$c_y(x, 1, t) = 1; \text{ for } \forall t \text{ and } 0 \leq x \leq 1, \quad (9d)$$

(iii) Initial condition:

(e) for the initial condition, we have:

$$c(x, y, 0) = 0; \text{ for } x \geq 0 \text{ and } y \geq 0. \quad (9e)$$

#### 3.1. Description of the Domain Using Finite Difference Scheme

For the finite difference method, we divide the domain of interest into different meshes of net sizes  $\Delta x$ ,  $\Delta y$  and  $\Delta t$  in the  $x$ ,  $y$ , and  $t$  directions respectively. Any node of the mesh can be represented as:

$$x_i = i\Delta x; i = 0, 1, 2, \dots, (I-1), \dots, n,$$

$$y_j = j\Delta y; j = 1, 2, \dots, (J-1), \dots, m,$$

$$t_k = k\Delta t; k = 1, 2, \dots,$$

wherein  $n\Delta x = 1$  and  $m\Delta y = 1$ . In the finite difference approximation, by applying the central, backward and forward finite differences for each partial derivative in Equation (9), we obtain different difference equations, which are an approximate solution of Equation (9). In this study, with application of some of these difference equations, we consider the consistency and stability of these equations because there is an important connection between the consistency of a stable finite difference scheme and the convergence of its solution to that of the partial differential equation it approximates. Lax's equivalence theorem [30] states that if a finite difference approximation to a well-posed linear initial

value problem is consistent, then stability is a necessary and sufficient condition for convergence. The two restrictions which apply to this theorem should be carefully noted. Firstly, the initial value problem must be well-posed; that is, the solution of the partial differential equation must depend continuously on the initial data. Secondly, the theorem only applies to linear problems. The important feature of linear equations is the sum of separate solutions are also a solution of the equation, which leads to the fact that the error terms themselves satisfy the homogeneous form of the finite difference equation which approximates the given differential equation. This theorem is of considerable practical importance. For while, it is relatively easy to show that a finite difference equation is stable and that it is consistent with a partial differential equation. It is usually very difficult to show that the solution of a finite difference equation converges to the solution of the partial differential equation that it approximates. Lax's equivalence theorem is needed to prove convergence in order to the finite difference approximation to the unsteady convective-diffusion Equation of (9), because the given differential equation is linear and is well-posed, it is sufficient to prove consistency and stability of the finite difference approximations of the Equation (9).

### 3.2. Appearance of Difference Equation by Application of Crank–Nicolson Method

For the partial derivatives in the Equation (9), we use central finite differences at the points  $(i\Delta x, j\Delta y, (k + \frac{1}{2})\Delta t)$  as follows:

$$\begin{aligned} c_t &= \frac{1}{\Delta t} (c_{i,j}^{k+1} - c_{i,j}^k) + O\{(\Delta t)^2\}, \\ c_y &= \frac{1}{2} \left[ \frac{c_{i,j+1}^k - c_{i,j-1}^k}{2\Delta y} + \frac{c_{i,j+1}^{k+1} - c_{i,j-1}^{k+1}}{2\Delta y} \right] + O\{(\Delta y)^2\}, \\ c_{xx} &= \frac{1}{2} \left[ \frac{c_{i+1,j}^k - 2c_{i,j}^k + c_{i-1,j}^k}{(\Delta x)^2} + \frac{c_{i+1,j}^{k+1} - 2c_{i,j}^{k+1} + c_{i-1,j}^{k+1}}{(\Delta x)^2} \right] + O\{(\Delta x)^2\}, \\ \text{and} \\ c_{yy} &= \frac{1}{2} \left[ \frac{c_{i,j+1}^k - 2c_{i,j}^k + c_{i,j-1}^k}{(\Delta y)^2} + \frac{c_{i,j+1}^{k+1} - 2c_{i,j}^{k+1} + c_{i,j-1}^{k+1}}{(\Delta y)^2} \right] + O\{(\Delta y)^2\}, \end{aligned}$$

we put these approximations in Equation (9):

$$\begin{aligned} & \frac{c_{i,j}^{k+1} - c_{i,j}^k}{\Delta t} + \frac{u}{2} \left[ \frac{c_{i,j+1}^k - c_{i,j-1}^k}{2\Delta y} + \frac{c_{i,j+1}^{k+1} - c_{i,j-1}^{k+1}}{2\Delta y} \right] \\ &= \frac{D}{2} \left[ \frac{c_{i+1,j}^k - 2c_{i,j}^k + c_{i-1,j}^k}{(\Delta x)^2} + \frac{c_{i+1,j}^{k+1} - 2c_{i,j}^{k+1} + c_{i-1,j}^{k+1}}{(\Delta x)^2} \right] \\ &+ \frac{D}{2} \left[ \frac{c_{i,j+1}^k - 2c_{i,j}^k + c_{i,j-1}^k}{(\Delta y)^2} + \frac{c_{i,j+1}^{k+1} - 2c_{i,j}^{k+1} + c_{i,j-1}^{k+1}}{(\Delta y)^2} \right]. \end{aligned}$$

Hence, we have:

$$\begin{aligned} & \frac{c_{i,j}^{k+1} - c_{i,j}^k}{\Delta t} + \frac{u}{4\Delta y} [(c_{i,j+1}^k - c_{i,j-1}^k) + (c_{i,j+1}^{k+1} - c_{i,j-1}^{k+1})] \\ &= \frac{D}{2(\Delta x)^2} [(c_{i+1,j}^k - 2c_{i,j}^k + c_{i-1,j}^k) + (c_{i+1,j}^{k+1} - 2c_{i,j}^{k+1} + c_{i-1,j}^{k+1})] \\ &+ \frac{D}{2(\Delta y)^2} [(c_{i,j+1}^k - 2c_{i,j}^k + c_{i,j-1}^k) + (c_{i,j+1}^{k+1} - 2c_{i,j}^{k+1} + c_{i,j-1}^{k+1})], \end{aligned}$$

which is the difference equation of Equation (9). By taking,  $p = \frac{(u\Delta t)}{\Delta y}$  and  $q = \frac{(D\Delta t)}{(\Delta x)^2} = \frac{(D\Delta t)}{(\Delta y)^2}$  wherein  $\Delta x = \Delta y$ , we have:

$$\begin{aligned} c_{i,j}^{k+1} - c_{i,j}^k + \frac{p}{4} [(c_{i,j+1}^k - c_{i,j-1}^k) + (c_{i,j+1}^{k+1} - c_{i,j-1}^{k+1})] \\ = \frac{q}{2} [(c_{i+1,j}^k - 2c_{i,j}^k + c_{i-1,j}^k) + (c_{i+1,j}^{k+1} - 2c_{i,j}^{k+1} + c_{i-1,j}^{k+1})] \\ + \frac{q}{2} [(c_{i,j+1}^k - 2c_{i,j}^k + c_{i,j-1}^k) + (c_{i,j+1}^{k+1} - 2c_{i,j}^{k+1} + c_{i,j-1}^{k+1})], \end{aligned}$$

wherein, we have:

$$\begin{aligned} 4c_{i,j}^{k+1} - 4c_{i,j}^k + p[(c_{i,j+1}^k - c_{i,j-1}^k) + (c_{i,j+1}^{k+1} - c_{i,j-1}^{k+1})] \\ = 2q[(c_{i+1,j}^k - 2c_{i,j}^k + c_{i-1,j}^k) + (c_{i+1,j}^{k+1} - 2c_{i,j}^{k+1} + c_{i-1,j}^{k+1})] \\ + 2q[(c_{i,j+1}^k - 2c_{i,j}^k + c_{i,j-1}^k) + (c_{i,j+1}^{k+1} - 2c_{i,j}^{k+1} + c_{i,j-1}^{k+1})], \end{aligned}$$

and

$$\begin{aligned} -2qc_{i-1,j}^{k+1} + (4 + 8q)c_{i,j}^{k+1} - 2qc_{i+1,j}^{k+1} = 2qc_{i-1,j}^k + (4 - 8q)c_{i,j}^k + 2qc_{i+1,j}^k \\ + p(c_{i,j-1}^k - c_{i,j+1}^k) + 2q(c_{i,j-1}^k + c_{i,j+1}^k) + p(c_{i,j-1}^{k+1} - c_{i,j+1}^{k+1}) \\ + 2q(c_{i,j-1}^{k+1} + c_{i,j+1}^{k+1}), \end{aligned} \quad (10)$$

where,  $i = 0, 1, \dots, n-1; j = 1, 2, \dots, m$  and  $k = 0, 1, 2, \dots$ . With application of the boundary and initial conditions, we have: with respect to Equation (9b) for each  $j$  and  $k$ , we have:

$$c_{n,j}^k = 1, \quad (11)$$

with respect to Equation (9c) for each  $i$  and  $k$ , we have:

$$c_{i,0}^k = 0. \quad (12)$$

Here, for numerical solution, we consider  $m=10$ . Therefore, by using central differences and with respect to Equation (9d), for each  $i$  and  $k$ , we have:

$$c_y = \frac{1}{2} \left[ \frac{c_{i,j+1}^k - c_{i,j-1}^k}{2\Delta y} + \frac{c_{i,j+1}^{k+1} - c_{i,j-1}^{k+1}}{2\Delta y} \right] + O\{(\Delta y)^2\},$$

and  $j = m = 10 \Rightarrow \Delta y = \frac{1}{m}, \Rightarrow \Delta y = 0.1$ . Thus,

$$1 = \frac{1}{2} \left[ \frac{c_{i,11}^k - c_{i,9}^k}{0.2} + \frac{c_{i,11}^{k+1} - c_{i,9}^{k+1}}{0.2} \right], \quad (13)$$

and

$$c_{i,11}^{k+1} + c_{i,11}^k = 0.4 + c_{i,9}^{k+1} + c_{i,9}^k; \quad (14)$$

where we use the terms  $c_{i,11}^{k+1} + c_{i,11}^k$  from Equation (14) in the numerical solution of Equation (9). With respect to Equation (9e) for each  $i$  and  $j$ , we have:

$$c_{i,j}^0 = 0, \quad (15)$$

and with respect to Equation (9a) for each  $j$  and  $k$ , we have:

$$c_x = \frac{1}{2} \left[ \frac{c_{i+1,j}^k - c_{i-1,j}^k}{2\Delta x} + \frac{c_{i+1,j}^{k+1} - c_{i-1,j}^{k+1}}{2\Delta x} \right] + O\{(\Delta x)^2\},$$

at  $i = 0$ , we have:

$$0 = \frac{1}{2} \left[ \frac{c_{1,j}^k - c_{-1,j}^k}{2\Delta x} + \frac{c_{1,j}^{k+1} - c_{-1,j}^{k+1}}{2\Delta x} \right],$$

and therefore,

$$c_{-1,j}^{k+1} + c_{-1,j}^k = c_{1,j}^{k+1} + c_{1,j}^k. \quad (16)$$

Now in Equation (10), we have:

$$\begin{aligned} -2qc_{-1,j}^{k+1} + (4 + 8q)c_{0,j}^{k+1} - 2qc_{1,j}^{k+1} &= 2qc_{-1,j}^k + (4 - 8q)c_{0,j}^k + 2qc_{1,j}^k \\ &+ p(c_{0,j-1}^k - c_{0,j+1}^k) + 2q(c_{0,j-1}^k + c_{0,j+1}^k) + p(c_{0,j-1}^{k+1} - c_{0,j+1}^{k+1}) + 2q(c_{0,j-1}^{k+1} + c_{0,j+1}^{k+1}), \end{aligned}$$

with application of Equation (16), we have:

$$\begin{aligned} -2q(c_{1,j}^{k+1} + c_{1,j}^k) + (4 + 8q)c_{0,j}^{k+1} - 2qc_{1,j}^{k+1} &= (4 - 8q)c_{0,j}^k + 2qc_{1,j}^k + p(c_{0,j-1}^k - c_{0,j+1}^k) \\ &+ 2q(c_{0,j-1}^k + c_{0,j+1}^k) + p(c_{0,j-1}^{k+1} - c_{0,j+1}^{k+1}) + 2q(c_{0,j-1}^{k+1} + c_{0,j+1}^{k+1}), \end{aligned}$$

wherein,

$$\begin{aligned} (4 + 8q)c_{0,j}^{k+1} - 4qc_{1,j}^{k+1} &= (4 - 8q)c_{0,j}^k + 4qc_{1,j}^k + p(c_{0,j-1}^k - c_{0,j+1}^k) \\ &+ 2q(c_{0,j-1}^k + c_{0,j+1}^k) + p(c_{0,j-1}^{k+1} - c_{0,j+1}^{k+1}) + 2q(c_{0,j-1}^{k+1} + c_{0,j+1}^{k+1}). \end{aligned} \quad (17)$$

Now by putting  $i = n - 1$ , in Equation (10), we have:

$$\begin{aligned} -2qc_{n-2,j}^{k+1} + (4 + 8q)c_{n-1,j}^{k+1} - 2qc_{n,j}^{k+1} &= 2qc_{n-2,j}^k + (4 - 8q)c_{n-1,j}^k + 2qc_{n,j}^k \\ &+ p(c_{n-1,j-1}^k - c_{n-1,j+1}^k) + 2q(c_{n-1,j-1}^k + c_{n-1,j+1}^k) \\ &+ p(c_{n-1,j-1}^{k+1} - c_{n-1,j+1}^{k+1}) + 2q(c_{n-1,j-1}^{k+1} + c_{n-1,j+1}^{k+1}), \end{aligned}$$

and with application of Equation (11), we have:

$$\begin{aligned} -2qc_{n-2,j}^{k+1} + (4 + 8q)c_{n-1,j}^{k+1} - 2q &= 2qc_{n-2,j}^k + (4 - 8q)c_{n-1,j}^k + 2q \\ &+ p(c_{n-1,j-1}^k - c_{n-1,j+1}^k) + 2q(c_{n-1,j-1}^k + c_{n-1,j+1}^k) \\ &+ p(c_{n-1,j-1}^{k+1} - c_{n-1,j+1}^{k+1}) + 2q(c_{n-1,j-1}^{k+1} + c_{n-1,j+1}^{k+1}), \end{aligned}$$

hence, we have:

$$\begin{aligned} -2qc_{n-2,j}^{k+1} + (4 + 8q)c_{n-1,j}^{k+1} &= 2qc_{n-2,j}^k + (4 - 8q)c_{n-1,j}^k + p(c_{n-1,j-1}^k - c_{n-1,j+1}^k) \\ &+ 2q(c_{n-1,j-1}^k + c_{n-1,j+1}^k) + p(c_{n-1,j-1}^{k+1} - c_{n-1,j+1}^{k+1}) \\ &+ 2q(c_{n-1,j-1}^{k+1} + c_{n-1,j+1}^{k+1}) + 4q. \end{aligned} \quad (18)$$

Now with application of Equations (10), (17) and (18), the matrix form of Equation (9) can be as follows:

$$\begin{aligned} Ac_{j,k+1} &= Bc_{j,k} + p[c_{j-1,k} - c_{j+1,k}] + 2q[c_{j-1,k} + c_{j+1,k}] \\ &+ p[c_{j-1,k+1} - c_{j+1,k+1}] + 2q[c_{j-1,k+1} + c_{j+1,k+1}] + d, \end{aligned} \quad (19)$$

where,  $A$  and  $B$  are square matrices of tri-diagonal dimensions of order  $n$  as follows:

$$A = \begin{bmatrix} 4+8q & -4q & & & \\ -2q & 4+8q & -2q & & \\ & \ddots & \ddots & \ddots & \\ & & -2q & 4+8q & -2q \\ & & & -2q & 4+8q \end{bmatrix},$$

and

$$B = \begin{bmatrix} 4-8q & 4q & & & \\ 2q & 4-8q & 2q & & \\ & \ddots & \ddots & \ddots & \\ & & 2q & 4-8q & 2q \\ & & & 2q & 4-8q \end{bmatrix},$$

$d$  and  $c_{j,k+1}$  are column vectors of order  $n$  as bellows:

$$d = [0, 0, \dots, 0, 4q]^T, \quad c_{j,k+1} = [c_{0,j}^{k+1}, c_{1,j}^{k+1}, \dots, c_{n-1,j}^{k+1}]^T,$$

132 wherein with the solution of this system by using Gauss elimination method or Gauss-Seidel method  
133 or Thomas algorithm, the  $c_{j,k+1}$  can be find.

### 134 3.3. The Truncation Error and Consistency

Difference equation of Equation (9) is as follows:

$$\begin{aligned} F_{i,j}^k(c) = & \frac{1}{\Delta t} (c_{i,j}^{k+1} - c_{i,j}^k) + \frac{u}{4\Delta y} \left[ (c_{i,j+1}^k - c_{i,j-1}^k) + (c_{i,j+1}^{k+1} - c_{i,j-1}^{k+1}) \right] \\ & - \frac{D}{2(\Delta x)^2} \left[ (c_{i+1,j}^k - 2c_{i,j}^k + c_{i-1,j}^k) + (c_{i+1,j}^{k+1} - 2c_{i,j}^{k+1} + c_{i-1,j}^{k+1}) \right] \\ & - \frac{D}{2(\Delta y)^2} \left[ (c_{i,j+1}^k - 2c_{i,j}^k + c_{i,j-1}^k) + (c_{i,j+1}^{k+1} - 2c_{i,j}^{k+1} + c_{i,j-1}^{k+1}) \right]. \end{aligned}$$



Since  $\Gamma_{i,j}^k = F_{i,j}^k(c)$ ; therefore by taking  $s = \Delta t$ ,  $r = \Delta y$  and  $h = \Delta x$  and applying Taylor series [30] about the point  $(i\Delta x, j\Delta y, k\Delta t)$ , we have:

$$\begin{aligned}
 *c_{i,j}^{k+1} &= c_{i,j}^k + s \frac{\partial c}{\partial t} \Big|_{i,j}^k + \frac{s^2}{2!} \frac{\partial^2 c}{\partial t^2} \Big|_{i,j}^k + \dots, \\
 *c_{i,j+1}^k &= c_{i,j}^k + r \frac{\partial c}{\partial y} \Big|_{i,j}^k + \frac{r^2}{2!} \frac{\partial^2 c}{\partial y^2} \Big|_{i,j}^k + \frac{r^3}{3!} \frac{\partial^3 c}{\partial y^3} \Big|_{i,j}^k + \dots, \\
 *c_{i,j-1}^k &= c_{i,j}^k - r \frac{\partial c}{\partial y} \Big|_{i,j}^k + \frac{r^2}{2!} \frac{\partial^2 c}{\partial y^2} \Big|_{i,j}^k - \frac{r^3}{3!} \frac{\partial^3 c}{\partial y^3} \Big|_{i,j}^k + \dots, \\
 *c_{i+1,j}^k &= c_{i,j}^k + h \frac{\partial c}{\partial x} \Big|_{i,j}^k + \frac{h^2}{2!} \frac{\partial^2 c}{\partial x^2} \Big|_{i,j}^k + \frac{h^3}{3!} \frac{\partial^3 c}{\partial x^3} \Big|_{i,j}^k + \dots, \\
 *c_{i-1,j}^k &= c_{i,j}^k - h \frac{\partial c}{\partial x} \Big|_{i,j}^k + \frac{h^2}{2!} \frac{\partial^2 c}{\partial x^2} \Big|_{i,j}^k - \frac{h^3}{3!} \frac{\partial^3 c}{\partial x^3} \Big|_{i,j}^k + \dots, \\
 \\
 *c_{i,j+1}^{k+1} &= c_{i,j}^k + s \frac{\partial c}{\partial t} \Big|_{i,j}^k + r \frac{\partial c}{\partial y} \Big|_{i,j}^k + \frac{s^2}{2!} \frac{\partial^2 c}{\partial t^2} \Big|_{i,j}^k + \frac{2sr}{2!} \frac{\partial^2 c}{\partial t \partial y} \Big|_{i,j}^k \\
 &\quad + \frac{r^2}{2!} \frac{\partial^2 c}{\partial y^2} \Big|_{i,j}^k + \frac{s^3}{3!} \frac{\partial^3 c}{\partial t^3} \Big|_{i,j}^k + \frac{3s^2 r}{3!} \frac{\partial^3 c}{\partial t^2 \partial y} \Big|_{i,j}^k + \frac{3sr^2}{3!} \frac{\partial^3 c}{\partial t \partial y^2} \Big|_{i,j}^k \\
 &\quad + \frac{r^3}{3!} \frac{\partial^3 c}{\partial y^3} \Big|_{i,j}^k + \frac{s^4}{4!} \frac{\partial^4 c}{\partial t^4} \Big|_{i,j}^k + \frac{r^4}{4!} \frac{\partial^4 c}{\partial y^4} \Big|_{i,j}^k + \dots, \\
 \\
 *c_{i,j-1}^{k+1} &= c_{i,j}^k + s \frac{\partial c}{\partial t} \Big|_{i,j}^k - r \frac{\partial c}{\partial y} \Big|_{i,j}^k + \frac{s^2}{2!} \frac{\partial^2 c}{\partial t^2} \Big|_{i,j}^k - \frac{2sr}{2!} \frac{\partial^2 c}{\partial t \partial y} \Big|_{i,j}^k \\
 &\quad + \frac{r^2}{2!} \frac{\partial^2 c}{\partial y^2} \Big|_{i,j}^k + \frac{s^3}{3!} \frac{\partial^3 c}{\partial t^3} \Big|_{i,j}^k - \frac{3s^2 r}{3!} \frac{\partial^3 c}{\partial t^2 \partial y} \Big|_{i,j}^k + \frac{3sr^2}{3!} \frac{\partial^3 c}{\partial t \partial y^2} \Big|_{i,j}^k \\
 &\quad - \frac{r^3}{3!} \frac{\partial^3 c}{\partial y^3} \Big|_{i,j}^k + \dots, \\
 \\
 *c_{i+1,j}^{k+1} &= c_{i,j}^k + s \frac{\partial c}{\partial t} \Big|_{i,j}^k + h \frac{\partial c}{\partial x} \Big|_{i,j}^k + \frac{s^2}{2!} \frac{\partial^2 c}{\partial t^2} \Big|_{i,j}^k + \frac{2sh}{2!} \frac{\partial^2 c}{\partial t \partial x} \Big|_{i,j}^k \\
 &\quad + \frac{h^2}{2!} \frac{\partial^2 c}{\partial x^2} \Big|_{i,j}^k + \frac{s^3}{3!} \frac{\partial^3 c}{\partial t^3} \Big|_{i,j}^k + \frac{3s^2 h}{3!} \frac{\partial^3 c}{\partial t^2 \partial x} \Big|_{i,j}^k + \frac{3sh^2}{3!} \frac{\partial^3 c}{\partial t \partial x^2} \Big|_{i,j}^k \\
 &\quad + \frac{h^3}{3!} \frac{\partial^3 c}{\partial x^3} \Big|_{i,j}^k + \dots, \\
 \\
 *c_{i-1,j}^{k+1} &= c_{i,j}^k + s \frac{\partial c}{\partial t} \Big|_{i,j}^k - h \frac{\partial c}{\partial x} \Big|_{i,j}^k + \frac{s^2}{2!} \frac{\partial^2 c}{\partial t^2} \Big|_{i,j}^k - \frac{2sh}{2!} \frac{\partial^2 c}{\partial t \partial x} \Big|_{i,j}^k \\
 &\quad + \frac{h^2}{2!} \frac{\partial^2 c}{\partial x^2} \Big|_{i,j}^k + \frac{s^3}{3!} \frac{\partial^3 c}{\partial t^3} \Big|_{i,j}^k - \frac{3s^2 h}{3!} \frac{\partial^3 c}{\partial t^2 \partial x} \Big|_{i,j}^k + \frac{3sh^2}{3!} \frac{\partial^3 c}{\partial t \partial x^2} \Big|_{i,j}^k \\
 &\quad - \frac{h^3}{3!} \frac{\partial^3 c}{\partial x^3} \Big|_{i,j}^k + \dots
 \end{aligned}
 \tag{20}$$

In the following expressions, we can find  $\Gamma_{i,j}^k$ .

$$\begin{aligned}
F_{i,j}^k(c) &= \frac{1}{s} [c_{i,j}^{k+1} - c_{i,j}^k] + \frac{u}{4r} \left[ (c_{i,j+1}^k - c_{i,j-1}^k) + (c_{i,j+1}^{k+1} - c_{i,j-1}^{k+1}) \right] \\
&\quad - \frac{D}{2h^2} \left[ (c_{i+1,j}^k - c_{i,j}^k) + (c_{i-1,j}^k - c_{i,j}^k) + (c_{i+1,j}^{k+1} - c_{i,j}^{k+1}) + (c_{i-1,j}^{k+1} - c_{i,j}^{k+1}) \right] \\
&\quad - \frac{D}{2r^2} \left[ (c_{i,j+1}^k - c_{i,j}^k) + (c_{i,j-1}^k - c_{i,j}^k) + (c_{i,j+1}^{k+1} - c_{i,j}^{k+1}) + (c_{i,j-1}^{k+1} - c_{i,j}^{k+1}) \right], \\
\\
\Rightarrow F_{i,j}^k(c) &= \frac{1}{s} (c_{i,j}^k + s \frac{\partial c}{\partial t} |_{i,j}^k + \frac{s^2}{2!} \frac{\partial^2 c}{\partial t^2} |_{i,j}^k + \frac{s^3}{3!} \frac{\partial^3 c}{\partial t^3} |_{i,j}^k + \dots - c_{i,j}^k) \\
&\quad + \frac{u}{4r} \left[ (c_{i,j}^k + r \frac{\partial c}{\partial y} |_{i,j}^k + \frac{r^2}{2!} \frac{\partial^2 c}{\partial y^2} |_{i,j}^k + \frac{r^3}{3!} \frac{\partial^3 c}{\partial y^3} |_{i,j}^k + \dots - c_{i,j}^k) \right. \\
&\quad - (c_{i,j}^k - r \frac{\partial c}{\partial y} |_{i,j}^k + \frac{r^2}{2!} \frac{\partial^2 c}{\partial y^2} |_{i,j}^k - \frac{r^3}{3!} \frac{\partial^3 c}{\partial y^3} |_{i,j}^k + \dots - c_{i,j}^k) \\
&\quad + (c_{i,j}^{k+1} + r \frac{\partial c}{\partial y} |_{i,j}^{k+1} + \frac{r^2}{2!} \frac{\partial^2 c}{\partial y^2} |_{i,j}^{k+1} + \frac{r^3}{3!} \frac{\partial^3 c}{\partial y^3} |_{i,j}^{k+1} + \dots - c_{i,j}^{k+1}) \\
&\quad - (c_{i,j}^{k+1} - r \frac{\partial c}{\partial y} |_{i,j}^{k+1} + \frac{r^2}{2!} \frac{\partial^2 c}{\partial y^2} |_{i,j}^{k+1} - \frac{r^3}{3!} \frac{\partial^3 c}{\partial y^3} |_{i,j}^{k+1} + \dots - c_{i,j}^{k+1}) \left. \right] \\
&\quad - \frac{D}{2h^2} \left[ (c_{i,j}^k + h \frac{\partial c}{\partial x} |_{i,j}^k + \frac{h^2}{2!} \frac{\partial^2 c}{\partial x^2} |_{i,j}^k + \frac{h^3}{3!} \frac{\partial^3 c}{\partial x^3} |_{i,j}^k + \dots - c_{i,j}^k) \right. \\
&\quad + (c_{i,j}^k - h \frac{\partial c}{\partial x} |_{i,j}^k + \frac{h^2}{2!} \frac{\partial^2 c}{\partial x^2} |_{i,j}^k - \frac{h^3}{3!} \frac{\partial^3 c}{\partial x^3} |_{i,j}^k + \dots - c_{i,j}^k) \\
&\quad + (c_{i,j}^{k+1} + h \frac{\partial c}{\partial x} |_{i,j}^{k+1} + \frac{h^2}{2!} \frac{\partial^2 c}{\partial x^2} |_{i,j}^{k+1} + \frac{h^3}{3!} \frac{\partial^3 c}{\partial x^3} |_{i,j}^{k+1} + \dots - c_{i,j}^{k+1}) \\
&\quad + (c_{i,j}^{k+1} - h \frac{\partial c}{\partial x} |_{i,j}^{k+1} + \frac{h^2}{2!} \frac{\partial^2 c}{\partial x^2} |_{i,j}^{k+1} - \frac{h^3}{3!} \frac{\partial^3 c}{\partial x^3} |_{i,j}^{k+1} + \dots - c_{i,j}^{k+1}) \left. \right] \\
&\quad - \frac{D}{2r^2} \left[ (c_{i,j}^k + r \frac{\partial c}{\partial y} |_{i,j}^k + \frac{r^2}{2!} \frac{\partial^2 c}{\partial y^2} |_{i,j}^k + \frac{r^3}{3!} \frac{\partial^3 c}{\partial y^3} |_{i,j}^k + \dots - c_{i,j}^k) \right. \\
&\quad + (c_{i,j}^k - r \frac{\partial c}{\partial y} |_{i,j}^k + \frac{r^2}{2!} \frac{\partial^2 c}{\partial y^2} |_{i,j}^k - \frac{r^3}{3!} \frac{\partial^3 c}{\partial y^3} |_{i,j}^k + \dots - c_{i,j}^k) \\
&\quad + (c_{i,j}^{k+1} + r \frac{\partial c}{\partial y} |_{i,j}^{k+1} + \frac{r^2}{2!} \frac{\partial^2 c}{\partial y^2} |_{i,j}^{k+1} + \frac{r^3}{3!} \frac{\partial^3 c}{\partial y^3} |_{i,j}^{k+1} + \dots - c_{i,j}^{k+1}) \\
&\quad + (c_{i,j}^{k+1} - r \frac{\partial c}{\partial y} |_{i,j}^{k+1} + \frac{r^2}{2!} \frac{\partial^2 c}{\partial y^2} |_{i,j}^{k+1} - \frac{r^3}{3!} \frac{\partial^3 c}{\partial y^3} |_{i,j}^{k+1} + \dots - c_{i,j}^{k+1}) \left. \right], \\
\\
\Rightarrow F_{i,j}^k(c) &= \frac{\partial c}{\partial t} |_{i,j}^k + \frac{s}{2!} \frac{\partial^2 c}{\partial t^2} |_{i,j}^k + \frac{s^2}{3!} \frac{\partial^3 c}{\partial t^3} |_{i,j}^k + \dots + \frac{u}{4} \left[ \frac{\partial c}{\partial y} |_{i,j}^k + \frac{r^2}{3!} \frac{\partial^3 c}{\partial y^3} |_{i,j}^k + \dots + \frac{\partial c}{\partial y} |_{i,j}^k + \frac{r^2}{3!} \frac{\partial^3 c}{\partial y^3} |_{i,j}^k + \dots \right. \\
&\quad + \frac{\partial c}{\partial y} |_{i,j}^{k+1} + \frac{r^2}{3!} \frac{\partial^3 c}{\partial y^3} |_{i,j}^{k+1} + \dots + \frac{\partial c}{\partial y} |_{i,j}^{k+1} + \frac{r^2}{3!} \frac{\partial^3 c}{\partial y^3} |_{i,j}^{k+1} + \dots \left. \right] - \frac{D}{2} \left[ \frac{1}{2} \frac{\partial^2 c}{\partial x^2} |_{i,j}^k + \frac{h^2}{4!} \frac{\partial^4 c}{\partial x^4} |_{i,j}^k + \dots \right. \\
&\quad + \frac{1}{2} \frac{\partial^2 c}{\partial x^2} |_{i,j}^k + \frac{h^2}{4!} \frac{\partial^4 c}{\partial x^4} |_{i,j}^k + \dots + \frac{1}{2} \frac{\partial^2 c}{\partial x^2} |_{i,j}^{k+1} + \frac{h^2}{4!} \frac{\partial^4 c}{\partial x^4} |_{i,j}^{k+1} + \dots \\
&\quad + \frac{1}{2} \frac{\partial^2 c}{\partial x^2} |_{i,j}^{k+1} + \frac{h^2}{4!} \frac{\partial^4 c}{\partial x^4} |_{i,j}^{k+1} + \dots \left. \right] - \frac{D}{2} \left[ \frac{1}{2} \frac{\partial^2 c}{\partial y^2} |_{i,j}^k + \frac{r^2}{4!} \frac{\partial^4 c}{\partial y^4} |_{i,j}^k + \dots + \frac{1}{2} \frac{\partial^2 c}{\partial y^2} |_{i,j}^k + \frac{r^2}{4!} \frac{\partial^4 c}{\partial y^4} |_{i,j}^k + \dots \right. \\
&\quad + \frac{1}{2} \frac{\partial^2 c}{\partial y^2} |_{i,j}^{k+1} + \frac{r^2}{4!} \frac{\partial^4 c}{\partial y^4} |_{i,j}^{k+1} + \dots + \frac{1}{2} \frac{\partial^2 c}{\partial y^2} |_{i,j}^{k+1} + \frac{r^2}{4!} \frac{\partial^4 c}{\partial y^4} |_{i,j}^{k+1} + \dots \left. \right],
\end{aligned}$$

$$\begin{aligned}
\Rightarrow F_{i,j}^k(c) = & \frac{\partial c}{\partial t}|_{i,j}^k + \frac{s}{2!} \frac{\partial^2 c}{\partial t^2}|_{i,j}^k + \frac{s^2}{3!} \frac{\partial^3 c}{\partial t^3}|_{i,j}^k + \dots + \frac{u}{4} \left[ \frac{\partial c}{\partial y}|_{i,j}^k + \frac{r^2}{3!} \frac{\partial^3 c}{\partial y^3}|_{i,j}^k + \dots + \frac{\partial c}{\partial y}|_{i,j}^k + \frac{r^2}{3!} \frac{\partial^3 c}{\partial y^3}|_{i,j}^k + \dots \right. \\
& + \left( \frac{\partial c}{\partial y}|_{i,j}^k + s \frac{\partial^2 c}{\partial t \partial y}|_{i,j}^k + \dots \right) + \frac{r^2}{3!} \left( \frac{\partial^3 c}{\partial y^3}|_{i,j}^k + s \frac{\partial^4 c}{\partial t \partial y^3}|_{i,j}^k + \dots \right) \\
& + \left( \frac{\partial c}{\partial y}|_{i,j}^k + s \frac{\partial^2 c}{\partial t \partial y}|_{i,j}^k + \dots \right) + \frac{r^2}{3!} \left( \frac{\partial^3 c}{\partial y^3}|_{i,j}^k + s \frac{\partial^4 c}{\partial t \partial y^3}|_{i,j}^k + \dots \right) \Big] - \frac{D}{2} \left[ \frac{1}{2} \frac{\partial^2 c}{\partial x^2}|_{i,j}^k + \frac{h^2}{4!} \frac{\partial^4 c}{\partial x^4}|_{i,j}^k + \dots \right. \\
& + \frac{1}{2} \frac{\partial^2 c}{\partial x^2}|_{i,j}^k + \frac{h^2}{4!} \frac{\partial^4 c}{\partial x^4}|_{i,j}^k + \dots + \frac{1}{2} \left( \frac{\partial^2 c}{\partial x^2}|_{i,j}^k + s \frac{\partial^3 c}{\partial t \partial x^2}|_{i,j}^k + \dots \right) + \frac{h^2}{4!} \left( \frac{\partial^4 c}{\partial x^4}|_{i,j}^k + s \frac{\partial^5 c}{\partial t \partial x^4}|_{i,j}^k + \dots \right) \\
& + \frac{1}{2} \left( \frac{\partial^2 c}{\partial x^2}|_{i,j}^k + s \frac{\partial^3 c}{\partial t \partial x^2}|_{i,j}^k + \dots \right) + \frac{h^2}{4!} \left( \frac{\partial^4 c}{\partial x^4}|_{i,j}^k + s \frac{\partial^5 c}{\partial t \partial x^4}|_{i,j}^k + \dots \right) \Big] - \frac{D}{2} \left[ \frac{1}{2} \frac{\partial^2 c}{\partial y^2}|_{i,j}^k + \frac{r^2}{4!} \frac{\partial^4 c}{\partial y^4}|_{i,j}^k + \dots \right. \\
& + \frac{1}{2} \frac{\partial^2 c}{\partial y^2}|_{i,j}^k + \frac{r^2}{4!} \frac{\partial^4 c}{\partial y^4}|_{i,j}^k + \dots \\
& + \frac{1}{2} \left( \frac{\partial^2 c}{\partial y^2}|_{i,j}^k + s \frac{\partial^3 c}{\partial t \partial y^2}|_{i,j}^k + \dots \right) + \frac{r^2}{4!} \left( \frac{\partial^4 c}{\partial y^4}|_{i,j}^k + s \frac{\partial^5 c}{\partial t \partial y^4}|_{i,j}^k + \dots \right) \\
& \left. + \frac{1}{2} \left( \frac{\partial^2 c}{\partial y^2}|_{i,j}^k + s \frac{\partial^3 c}{\partial t \partial y^2}|_{i,j}^k + \dots \right) + \frac{r^2}{4!} \left( \frac{\partial^4 c}{\partial y^4}|_{i,j}^k + s \frac{\partial^5 c}{\partial t \partial y^4}|_{i,j}^k + \dots \right) \right],
\end{aligned}$$

$$\begin{aligned}
\Rightarrow F_{i,j}^k(c) = & \frac{\partial c}{\partial t}|_{i,j}^k + \frac{s}{2!} \frac{\partial^2 c}{\partial t^2}|_{i,j}^k + \frac{s^2}{3!} \frac{\partial^3 c}{\partial t^3}|_{i,j}^k \\
& + \frac{u}{4} \left\{ 4 \frac{\partial c}{\partial y}|_{i,j}^k + 2s \frac{\partial^2 c}{\partial t \partial y}|_{i,j}^k + \frac{4r^2}{3!} \left( \frac{\partial^3 c}{\partial y^3}|_{i,j}^k + \frac{2r^2}{3!} \left( 2s \frac{\partial^4 c}{\partial t \partial y^3}|_{i,j}^k \right) \right) \right\} \\
& - \frac{D}{2} \left\{ 2 \frac{\partial^2 c}{\partial x^2}|_{i,j}^k + s \frac{\partial^3 c}{\partial t \partial x^2}|_{i,j}^k + \frac{h^2}{3!} \frac{\partial^4 c}{\partial x^4}|_{i,j}^k + 2 \frac{h^2}{4!} s \frac{\partial^5 c}{\partial t \partial x^4}|_{i,j}^k \right\} \\
& - \frac{D}{2} \left\{ 2 \frac{\partial^2 c}{\partial y^2}|_{i,j}^k + s \frac{\partial^3 c}{\partial t \partial y^2}|_{i,j}^k + \frac{r^2}{3!} \frac{\partial^4 c}{\partial y^4}|_{i,j}^k + 2 \frac{r^2}{4!} s \frac{\partial^5 c}{\partial t \partial y^4}|_{i,j}^k \right\},
\end{aligned}$$

$$\begin{aligned}
\Rightarrow F_{i,j}^k(c) = & \frac{\partial c}{\partial t}|_{i,j}^k + u \frac{\partial c}{\partial y}|_{i,j}^k - D \frac{\partial^2 c}{\partial x^2}|_{i,j}^k - D \frac{\partial^2 c}{\partial y^2}|_{i,j}^k + \frac{s}{2} \frac{\partial^2 c}{\partial t^2}|_{i,j}^k \\
& + \frac{s}{2} u \frac{\partial^2 c}{\partial t \partial y}|_{i,j}^k - \frac{s}{2} D \frac{\partial^3 c}{\partial t \partial x^2}|_{i,j}^k - \frac{s}{2} D \frac{\partial^3 c}{\partial t \partial y^2}|_{i,j}^k + \frac{s^2}{3!} \frac{\partial^3 c}{\partial t^3}|_{i,j}^k \\
& + \frac{u}{4} \left( \frac{4r^2}{3!} \frac{\partial^3 c}{\partial y^3}|_{i,j}^k + \frac{4r^2}{4!} s \frac{\partial^4 c}{\partial t \partial y^3}|_{i,j}^k \right) \\
& - \frac{D}{2} \left( \frac{h^2}{3!} \frac{\partial^4 c}{\partial x^4}|_{i,j}^k + \frac{2h^2}{4!} s \frac{\partial^5 c}{\partial t \partial x^4}|_{i,j}^k \right) - \frac{D}{2} \left( \frac{r^2}{3!} \frac{\partial^4 c}{\partial y^4}|_{i,j}^k \right. \\
& \left. + \frac{2r^2}{4!} s \frac{\partial^5 c}{\partial t \partial y^4}|_{i,j}^k \right),
\end{aligned}$$

with respect to Equation (9), we have:

$$\frac{\partial c}{\partial t} + u \frac{\partial c}{\partial y} - D \frac{\partial^2 c}{\partial x^2} - D \frac{\partial^2 c}{\partial y^2} = 0.$$

And by obtaining derivative with respect to time  $t$ , we have:

$$\frac{\partial^2 c}{\partial t^2} + u \frac{\partial^2 c}{\partial t \partial y} - D \frac{\partial^3 c}{\partial t \partial x^2} - D \frac{\partial^3 c}{\partial t \partial y^2} = 0,$$

therefore, we have:

$$F_{i,j}^k(c) = \frac{s^2}{3!} \frac{\partial^3 c}{\partial t^3} \Big|_{i,j}^k + u \left( \frac{r^2}{3!} \frac{\partial^3 c}{\partial y^3} \Big|_{i,j}^k + \frac{r^2}{3!} s \frac{\partial^4 c}{\partial t \partial y^3} \Big|_{i,j}^k \right) \\ - D \left( \frac{h^2}{3!} \frac{\partial^4 c}{\partial x^4} \Big|_{i,j}^k + \frac{2h^2}{4!} s \frac{\partial^5 c}{\partial t \partial x^4} \Big|_{i,j}^k \right) - D \left( \frac{r^2}{3!} \frac{\partial^4 c}{\partial y^4} \Big|_{i,j}^k + \frac{2r^2}{4!} s \frac{\partial^5 c}{\partial t \partial y^4} \Big|_{i,j}^k \right).$$

Hence, the introduced difference equation is consistent with the unsteady convective-diffusion (in both directions) partial differential Equation (9) and has the error of order of  $O((\Delta t)^2 + (\Delta x)^2 + (\Delta y)^2)$  wherein we want to achieve.

### 3.4. Stability of the Mathematical Model

With respect to the matrix form of Equation (19) and the boundary conditions on  $y$ , we have:

$$-(-p + 2q)c_{j+1}^{k+1} + Ac_j^{k+1} - (p + 2q)c_{j-1}^{k+1} = (-p + 2q)c_{j+1}^k + Bc_j^k + (p + 2q)c_{j-1}^k + d, \quad (21)$$

for  $j = 2, 3, \dots, m - 2$ ; and in  $j = 1$ , we have:

$$-(-p + 2q)c_2^{k+1} + Ac_1^{k+1} = (-p + 2q)c_2^k + Bc_1^k + d, \quad (22)$$

and in  $j = m - 1$ , we have:

$$\frac{1}{2} \left( \frac{c_m^{k+1} - c_{m-2}^{k+1}}{2\Delta y} \right) + \frac{1}{2} \left( \frac{c_m^k - c_{m-2}^k}{2\Delta y} \right) = 1.$$

Hence,

$$Ac_{m-1}^{k+1} - 4qc_{m-2}^{k+1} = Bc_{m-1}^k + 4qc_{m-2}^k + d + (-p + 2q)4\Delta y. \quad (23)$$

The relations (21), (22) and (23) in matrix form can be written as follows:

$$Mc^{k+1} = Nc^k + Q,$$

where,

$$M = \begin{bmatrix} A & (p-2q)I & & & \\ -(p+2q)I & A & (p-2q)I & & \\ & \ddots & \ddots & \ddots & \\ & & -(p+2q)I & A & (p-2q)I \\ & & & -4qI & A \end{bmatrix}_{m^2 \times m^2},$$

$$c^{k+1} = \left[ c_{1,1}^{k+1}, c_{2,1}^{k+1}, \dots, c_{m,1}^{k+1}, c_{1,2}^{k+1}, c_{2,2}^{k+1}, \dots, c_{m,2}^{k+1}, \dots, c_{m,m}^{k+1} \right]_{m^2 \times 1}^T,$$

$$c^k = \left[ c_{1,1}^k, c_{2,1}^k, \dots, c_{m,1}^k, c_{1,2}^k, c_{2,2}^k, \dots, c_{m,2}^k, \dots, c_{m,m}^k \right]_{m^2 \times 1}^T,$$

$$N = \begin{bmatrix} B & (-p+2q)I & & & \\ (p+2q)I & B & (-p+2q)I & & \\ & \ddots & \ddots & \ddots & \\ & & (p+2q)I & B & (-p+2q)I \\ & & & (p+2q)I & B \end{bmatrix}_{m^2 \times m^2};$$

Under matrix  $Q$ :

$$Q = \begin{bmatrix} d \\ d \\ \vdots \\ d+f \end{bmatrix}_{m^2 \times 1},$$

and  $f = 4(-p+2q)\Delta y I$ . With respect to the stability concept by [32], here we pursue the suitable stability condition for the above difference equation. Suppose at first, for a small perturbation, we put  $c_*^{k+1}$  instead of  $c^{k+1}$  and  $c_*^k$  instead of  $c^k$ . Then, we consider:

$$M(c^{k+1} - c_*^{k+1}) = N(c^k - c_*^k) + Q - Q;$$

For,  $e^{k+1} = c^{k+1} - c_*^{k+1}$ , we have:  $Me^{k+1} = Ne^k$ ; therefore,  $e^{k+1} = M^{-1}Ne^k$ ; hence,  $\|e^{k+1}\|_1 = \|M^{-1}Ne^k\|_1 \leq \|M^{-1}N\|_1 \|e^k\|_1 = \|M^{-1}N\|_1^{k+1} \|e^0\|_1$ ; also, we have:  $\|M^{-1}N\|_1 \leq \|M^{-1}\|_1 \|N\|_1$  (we take  $\|\cdot\|_1$  [33]). Since matrix  $M$  is strictly diagonally dominant, it is invertible and  $\|M^{-1}\|_1 \neq 0$ . Define  $T = \frac{M}{\|M+I\|_1}$ ,  $\|T\|_1 \leq 1$ . Obviously, we have:  $\|M+I\|_1 \neq 0$  (wherein  $\|M+I\|_1 = p+2q+3$ ),

$$\begin{aligned} [I - (T-I)T^{-1}][I + T - I] &= I, \\ \|T^{-1}\|_1 &= \|I - (T-I)T^{-1}\|_1 \leq \|I\|_1 + \|T-I\|_1 \|T^{-1}\|_1, \end{aligned}$$

$$(1 - \|T-I\|_1) \|T^{-1}\|_1 \leq 1; (\|T-I\|_1 \leq 1) \longrightarrow \|T^{-1}\|_1 \leq \frac{1}{1 - \|T-I\|_1}.$$

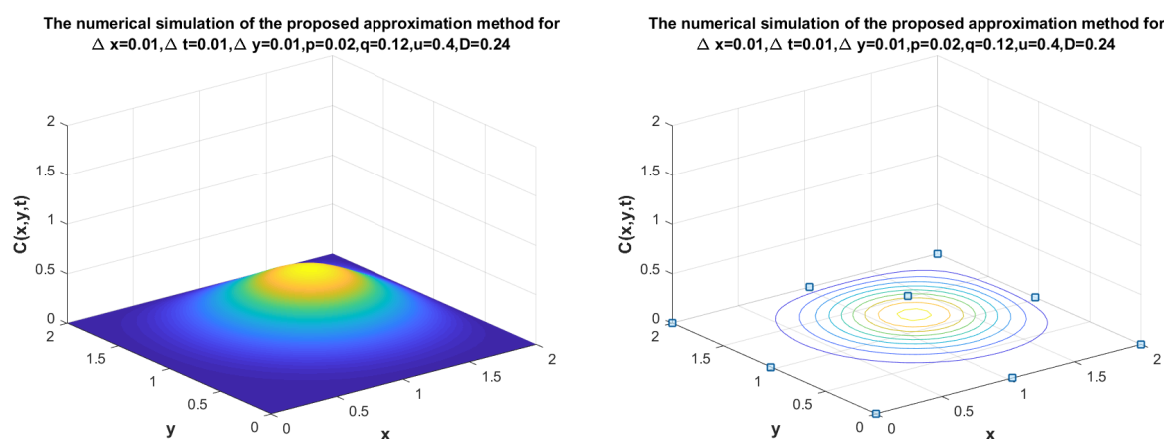
Now, by substitution of  $\frac{M}{\|M+I\|_1}$ , we have:

$$\|(\frac{M}{\|M+I\|_1})^{-1}\|_1 = \|M+I\|_1 \|M^{-1}\|_1 \leq \frac{1}{1 - \|\frac{M}{\|M+I\|_1} - I\|_1};$$

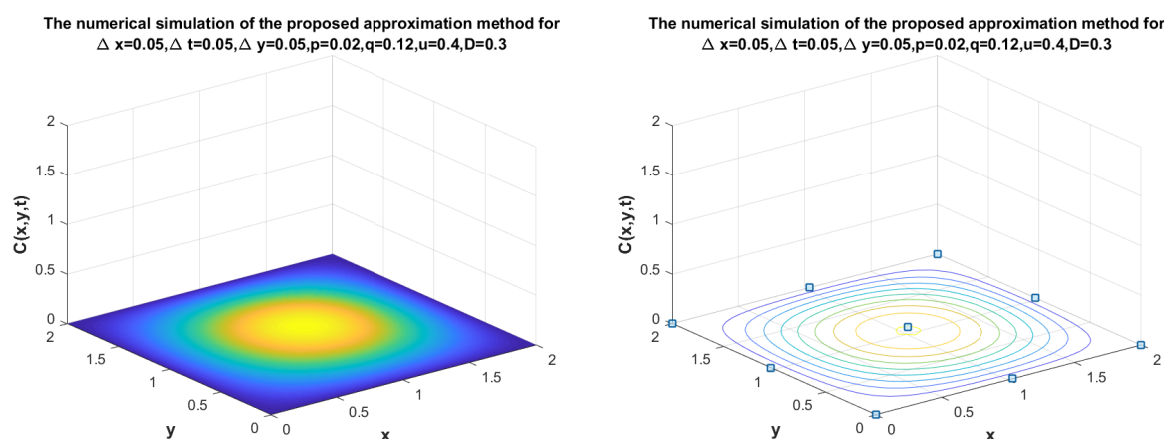
$$\Rightarrow \|M^{-1}\|_1 \leq \frac{1}{\|M+I\|_1 - \|M - \|M+I\|_1 I\|_1};$$

$$\begin{aligned} \Rightarrow \|M^{-1}\|_1 \|N\|_1 &\leq \frac{\|N\|_1}{\|M+I\|_1 - \|M - \|M+I\|_1 I\|_1} \\ &\leq \frac{4+14q+2p}{4+18q+2p} < 1. \end{aligned}$$

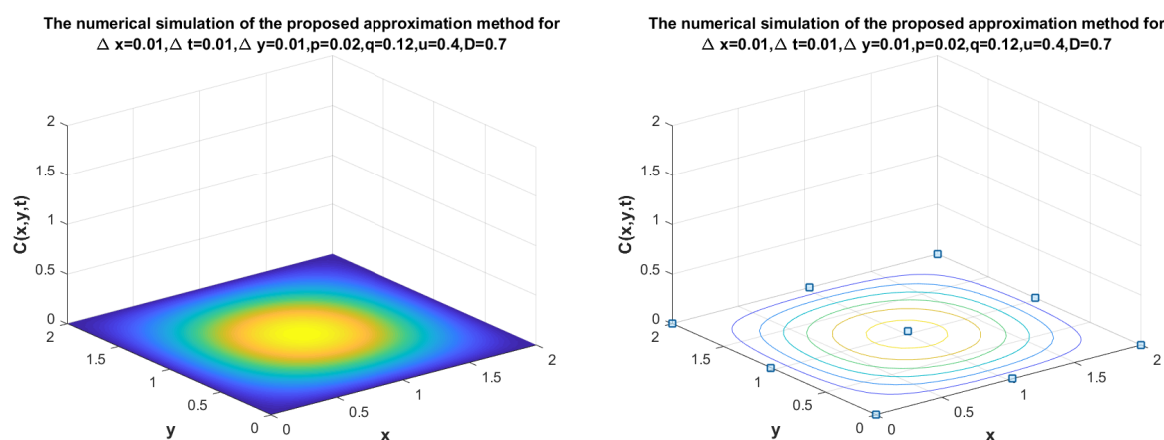
139 Hence, for real and positive values of  $p$  and  $q$ , the difference scheme is unconditionally stable.  
140 This means that for each  $\Delta t$ ,  $\Delta x$  and  $\Delta y$ , the difference scheme is unconditionally stable.



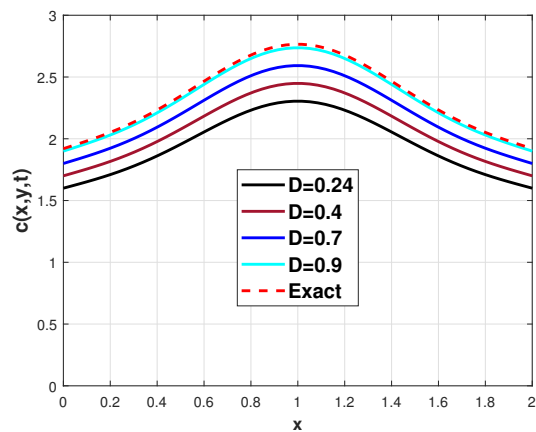
**Figure 1.** The numerical simulation of the proposed approximation method for equation (9) with  $\Delta x = 0.01, \Delta t = 0.01, \Delta y = 0.01, p = 0.02, q = 0.12, u = 0.4, D = 0.24$



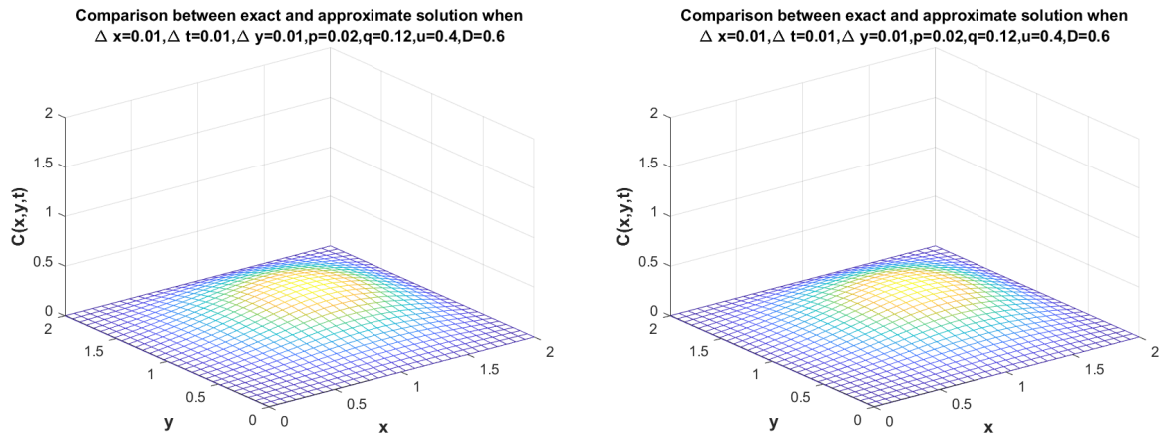
**Figure 2.** The numerical simulation of the proposed approximation method for equation (9) with  $\Delta x = 0.05, \Delta t = 0.05, \Delta y = 0.05, p = 0.02, q = 0.12, u = 0.4, D = 0.3$



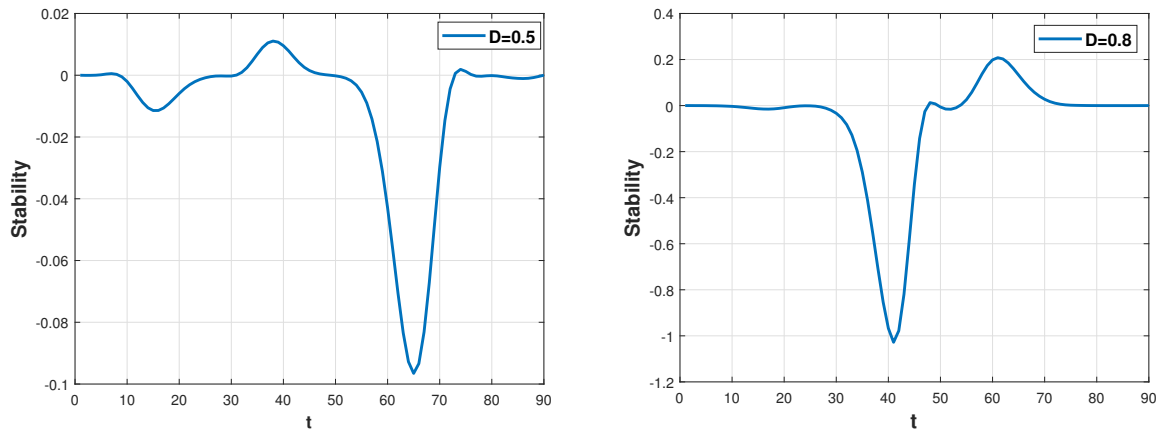
**Figure 3.** The numerical simulation of the proposed approximation method for equation (9) with  $\Delta x = 0.01, \Delta t = 0.01, \Delta y = 0.01, p = 0.02, q = 0.12, u = 0.4, D = 0.7$



**Figure 4.** The comparison of the obtained solutions of the proposed approximation method and exact solution for equation (9) with various values of  $D$ .



**Figure 5.** Comparison between exact and approximate solution for equation (9) with various values of  $D$ .



**Figure 6.** Stability of the approximate solution for equation (9) with various values of  $D$ .

#### 141 4. Numerical Investigation of the Present Study

142 In the present study, the unsteady convective-diffusion (in the both directions) partial differential  
 143 equation (9) together with the boundary (9a, b), entrance (9c, d) and initial (9e) conditions is solved  
 144 numerically by the finite difference scheme. For this, the first order derivative in time is approximated  
 145 by the second order difference formula and the diffusion terms in axial and radial directions is  
 146 expressed by the second order Crank-Nicolson difference operator. On one hand, the approximation of  
 147 convective term in the governing equation by central differences provides the non-physical oscillation  
 148 in the solution. On the other hand, upwind finite difference scheme gives the solution free from  
 149 the oscillation but it reduces the accuracy of the solution. Thus, for retaining the second order  
 150 accuracy of the solution for convective term, the Crank-Nicolson second order accuracy of the finite  
 151 difference scheme is used to approximate the convective term which provides the solution free from  
 152 the oscillations. The finite difference formulation leads to a system of linear algebraic equations which  
 153 needs a technique for computing the solution. It may be noted that the system has the tri-diagonal  
 154 character [34]. Such a system can be solved by the point iterative methods. However, the convergence  
 155 of the point iterative methods is very slow. In order to achieve faster convergence, we can use the line  
 156 iterative method. This method uses the tri-diagonal character of the coefficient matrix of equation, and  
 157 is easy to solve by the Thomas algorithm. Further, it may be noted that, by using this technique, the  
 158 equation involves an unknown  $c$  at every row for a fixed time level which saves the storage on the  
 159 computer. According to the Lax's equivalence theorem, mathematical proofs of the numerical solution  
 160 technique were obtained. Hence, the consistency and stability of the equations were investigated which  
 161 assure the convergences. Computations have been done for ten intervals with  $x=0.1$  in the positive  
 162  $x$  direction, the step size  $y=0.1$  in the positive  $y$  direction and the time step  $t=0.05$  in the positive  $t$   
 163 direction. The programs were tested even for the smaller step sizes. The technique described here can  
 164 be used to solve any linear system of unsteady convective-diffusion partial differential equation where  
 165 the axial diffusion term is ignored. Further, we may point out that the technique works in the equations  
 166 including axial diffusion term as well wherein we have done here in the form of the equation(9).

#### 167 5. Numerical results

168 In this section, we show the numerical simulation of the proposed approximation method for  
 169 various values of  $D, u, \Delta x, \Delta y, \Delta t, p, q$  to verify the efficiency of the proposed numerical method. The  
 170 numerical simulation of the proposed approximation method in Figures 1 to 4 are shown. The  
 171 behaviour of the obtained error for different values of  $D$  are presented in Figure 5. In Figure 6 stability  
 172 of the approximate solution for equation (9) with various values of  $D$  are presented.

#### 173 6. Conclusions

174 In the present study, we have considered a mathematical model for studying the non-steady  
 175 transport of oxygen in a slab of capillary. The capillary is assumed to be a two-dimensional channel  
 176 in dimensionless form. We have found that the difference equation which is described here, has the  
 177 same higher order of accuracy, wherein we want to achieve. We have increased the order of accuracy  
 178 from our previous study  $O[(\Delta t) + (\Delta y) + (\Delta x)^2]$  [35], to the present higher order scheme using the  
 179 Crank-Nicolson method, i.e.,  $O[(\Delta t)^2 + (\Delta x)^2 + (\Delta y)^2]$ . For stability condition, we have seen that, the  
 180 equations presented in the previous sections, are all stable and the results converges well. Further,  
 181 numerical results show that the axial diffusion does not effect the process of the oxygenation in a slab  
 182 of the capillary.

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## References

1. Wu, W.T.; Li, Y.; Aubry, N.; Massoudi, M.; Antaki, J.F. Numerical simulation of red blood cell-induced platelet transport in saccular aneurysms. *Appl. Sci.* **2017**, *7*, 484.
2. Bridges, C.; Karra, S.; Rajagopal, K.R. On modelling the response of the synovial fluid: Unsteady flow of a shear-thinning, chemically-reacting fluid mixture. *Comput. Math. Appl.* **2010**, *60*, 2333.
3. Hund, S.J.; Antaki, J.F. An extended convection diffusion model for red blood cell-enhanced transport of thrombocytes and leukocytes. *Phys. Med. Biol.* **2009**, *54*, 6415.
4. Wu, W.T.; Massoudi, M. Heat transfer and dissipation effects in the flow of a drilling fluid. *Fluids* **2016**, *1*, 4.
5. Massoudi, M.; Antaki, J. An anisotropic constitutive equation for the stress tensor of blood based on mixture theory. *Math. Probl. Eng.*, doi:10.1155/2008/579172.
6. Skrzeczewski, T.; Erickson, L.C.; Fogelson, A.L. Platelet motion near a vessel wall or thrombus surface in two-dimensional whole blood simulations. *Biophysical J.* **2013**, *104*, 1764.
7. Burger, J.M. Numerical study on non-linear Burger's and modified Burger's equations using B-Splines. Internet Connection.
8. Zhan, W.; Wang, C.H. Convection enhanced delivery of chemotherapeutic drugs into brain tumour. *J. Control. Release* **2018**, *271*, 74.
9. Kaesler, A.; Rosen, M.; Schmitz-Rode, T.; Steinseifer, U.; Arens, J. Computational modelling of oxygen transfer in artificial lungs. *Artif. Organs* **2018**, doi:10.1111/aor.13146.
10. Melnik, R.V.N.; Jenkins, D.R. On computational control of flow in airblast atomisers for pulmonary drug delivery. *Int. J. Pharm.* **2002**, *239*, 23.
11. Mountrakis, L.; Lorenz, E.; Hoekstra, A.G. Where do the platelets go? A simulation study of fully resolved blood flow through aneurysmal vessels. *Interface Focus* **2013**, doi:10.1098/rsfs.2012.0089.
12. Whittle, I.R.; Dorsch, N.W.; Besser, M. Spontaneous thrombosis in giant intracranial aneurysms. *J. Neurol. Neurosurg. Psychiatry* **1982**, *45*, 1040.
13. Hirabayashi, M.; Ohta, M.; Rüfenacht, D.A.; Chopard, B. Characterization of flow reduction properties in an aneurysm due to a stent. *Phys. Rev. E* **2003**, *68*, 021918.
14. Weir, B. Unruptured intracranial aneurysms: A review. *J. Neurosurg.* **2002**, *96*, 3.
15. Desai, C.S.; Johnson, L.D. Evaluation of some numerical schemes for consolidation. *Int. J. Numer. Methods Eng.* **1973**, *7*, 243.
16. Aminataei, A.; Sharan, M.; Singh, M.P. A numerical solution for the non-linear convective facilitated diffusion reaction problem for the process of blood oxygenation in the lungs. *J. Nat. Acad. Math.* **1985**, *3*, 182.
17. Aminataei, A.; Sharan, M.; Singh, M.P. A numerical model for the process of gas exchange in the pulmonary capillaries. *Ind. J. Pure. Appl. Math.* **1987**, *18*, 1040.
18. Aminataei, A.; Sharan, M.; Singh, M.P. Two layer model for the process of blood oxygenation in the pulmonary capillaries-parabolic profiles in the core as well as in the plasma layer. *Appl. Math. Modelling.* **1988**, *12*, 601.
19. Aminataei, A. A numerical two layer model for blood oxygenation in lungs. *Amir-Kabir J. Sci. Tech.* **2001**, *12*, 63.
20. A. Aminataei, Comparison of explicit and implicit approaches to numerical solution of uni-dimensional equation of diffusion, *J. of Sci., Al-Zahra Univ.* **2002**, *1*, 15.
21. A. Aminataei, Blood oxygenation in the pulmonary circulation: a review, *Euro. J. Scien. Res.* **2005**, *10*, 55.
22. A. Aminataei, A numerical simulation of the unsteady convective-diffusion equation, *The J. of Damghan Univ. of Basic Scis.* **2008**, *1*, 73.
23. A. Aminataei and S. Hassani, An efficient numerical method for the solution of initial and boundary values problems, *J. of Sci., Al-Zahra Univ.* **2009**, *22*, 13.
24. E.F. Leonard and S.B. Jørgensen, The analysis of convection and diffusion in capillary beds, *Annu. Rev. Biophys. Bioeng.* **1974**, *3*, 293.
25. A. Aminataei, Simulation of the breathing gases in the airways, *J. Advan. Math. Model.* **2012**, *1*, 51.
26. Aminataei, A. A mathematical model for oxygen dissociation curve in the blood. *Eur. J. Sci. Res.* **2005**, *6*, 5.
27. Lapidus, L.; Pinder, G.F. *Numerical Solution of Partial Differential Equations in Science and Engineering*; John Wiley & Sons: New York, NY, USA, 1982.
28. Aminataei, A. The study of diffusion equation in the pulmonary circulation. *J. Maths. Soc.* **2014**, *1*, 17.

- 237 29. Sharan, M.; Singh, M.P.; Aminataei, A. A numerical model for blood oxygenation in the pulmonary  
238 capillaries-effect of pulmonary membrane resistance. *BioSystems* **1987**, *20*, 355.
- 239 30. Lax, P.D.; Richtmyer, R.D. Survey of the stability of linear finite difference equations. *Commun. Pure Appl.*  
240 *Math.* **1959**, *9*, 267.
- 241 31. Evans, G.; Blackledge, J.; Yardleg, P. *Numerical Methods for Partial Differential Equations*; Springer-Verlag:  
242 London, UK, 2000.
- 243 32. Smith, G.D. *Numerical Solution of Partial Differential Equations: Finite Difference Methods*; Oxford University  
244 Press: Oxford, UK, 1993.
- 245 33. Noye, J. *Numerical Simulation of Fluid Motion*; North-Holland: Amsterdam, The Netherlands, 1978.
- 246 34. Thomas, L.H. *Elliptic Problems in Linear Difference Equations Over a Network*. Watson Scientific Computing  
247 Laboratory, New York, Columbia University, 1949.
- 248 35. Aminataei, A. Numerical simulation of the process of oxygen mass transport in the human pulmonary  
249 capillaries incorporating the contribution of axial diffusion. *J. Sci. Kharazmi Univ.* **2013**, *13*, 779.