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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.

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

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

67 2. Mathematical Description of the Model as a Whole

68 Let us consider at first, the RBC distribution and the blood flow transport. When we have
 69 succeeded, we can add aneurysms wherein it has been described in the different literature in
 70 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 carbon dioxide) at the position p and the time t . Position p in Cartesian co-ordinate is (x, y, ζ) or in polar co-ordinate is (r, θ, ζ) 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 α) 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:

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

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

89 **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:

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

90 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
 91 uniform with an average velocity $u = 0.4$, and the diffusion coefficient of oxygen is considered as a
 92 constant quantity, $D = 0.24$. The first and second terms on the left-side are respectively the rate of
 93 change of concentration per unit time and the transport due to convection whereas the terms on the
 94 right-side indicate the free molecular diffusion in the radial as well as axial directions. Equation (9) is
 95 to be solved under the following boundary, entrance and initial conditions.

96 (i) Boundary conditions:

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

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

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

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

101 (ii) Entrance conditions:

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

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

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

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

106 (iii) Initial condition:

107 (e) for the initial condition, we have:

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

109 *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 Δx , Δy and Δt in the x , y , and t directions respectively. Any node of the mesh can be represented as:

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

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

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

110 wherein $n\Delta x = 1$ and $m\Delta y = 1$. In the finite difference approximation, by applying the central,
 111 backward and forward finite differences for each partial derivative in Equation (9), we obtain different
 112 difference equations, which are an approximate solution of Equation (9). In this study, with application
 113 of some of these difference equations, we consider the consistency and stability of these equations
 114 because there is an important connection between the consistency of a stable finite difference scheme
 115 and the convergence of its solution to that of the partial differential equation it approximates. Lax's
 116 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:

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

and

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

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:

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

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:

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

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:

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

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

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

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

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:

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

¹³⁵ Hence, the introduced difference equation is consistent with the unsteady convective-diffusion (in both
¹³⁶ directions) partial differential Equation (9) and has the error of order of $O((\Delta t)^2 + (\Delta x)^2 + (\Delta y)^2)$
¹³⁷ wherein we want to achieve.

¹³⁸ *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,

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

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

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

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

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 Δt , Δx and Δy , the difference scheme is unconditionally stable.

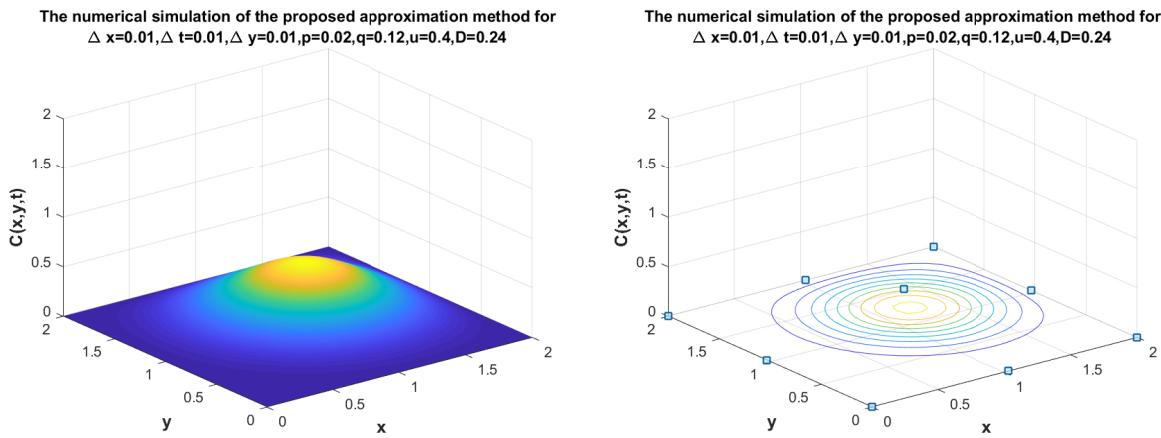


Figure 1. The numerical simulation of the proposed approximation method for equation (9) with $\Delta x = 0.01, \Delta t = 0.01, \Delta y = 0.01, p = 0.02, q = 0.12, u = 0.4, D = 0.24$

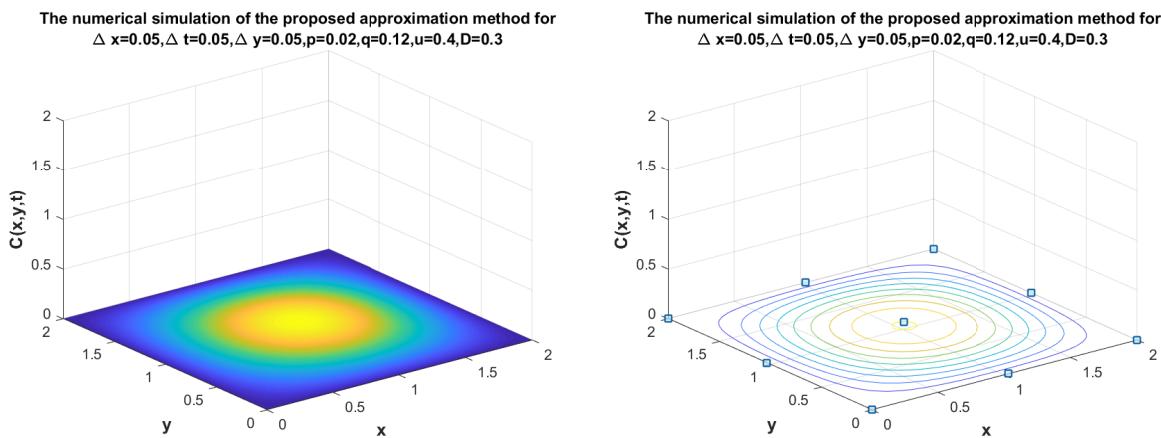


Figure 2. The numerical simulation of the proposed approximation method for equation (9) with $\Delta x = 0.05, \Delta t = 0.05, \Delta y = 0.05, p = 0.02, q = 0.12, u = 0.4, D = 0.3$

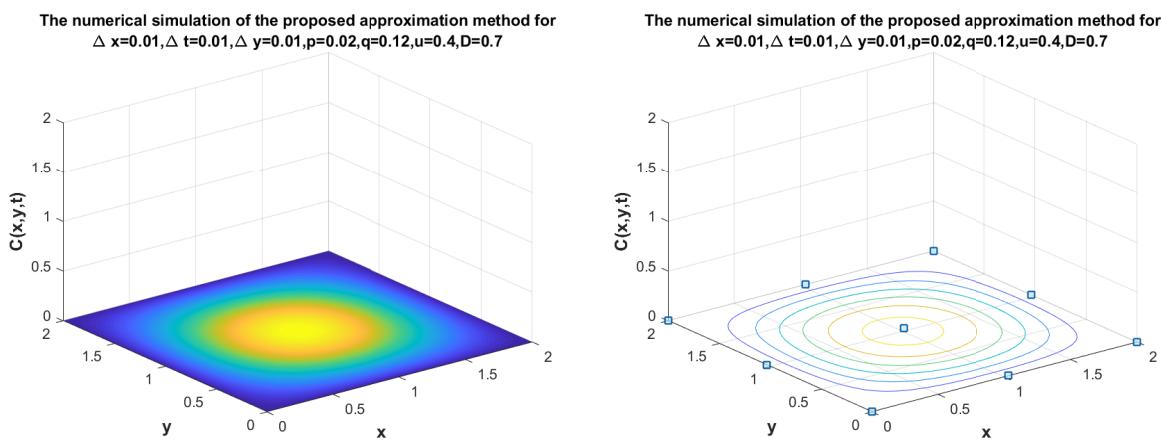


Figure 3. The numerical simulation of the proposed approximation method for equation (9) with $\Delta x = 0.01, \Delta t = 0.01, \Delta y = 0.01, p = 0.02, q = 0.12, u = 0.4, D = 0.7$

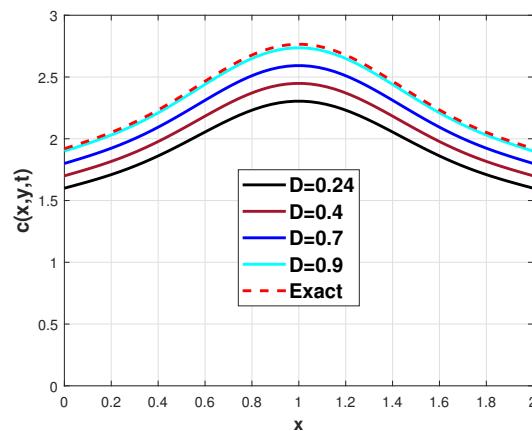


Figure 4. The comparison of the obtained solutions of the proposed approximation method and exact solution for equation (9) with various values of D .

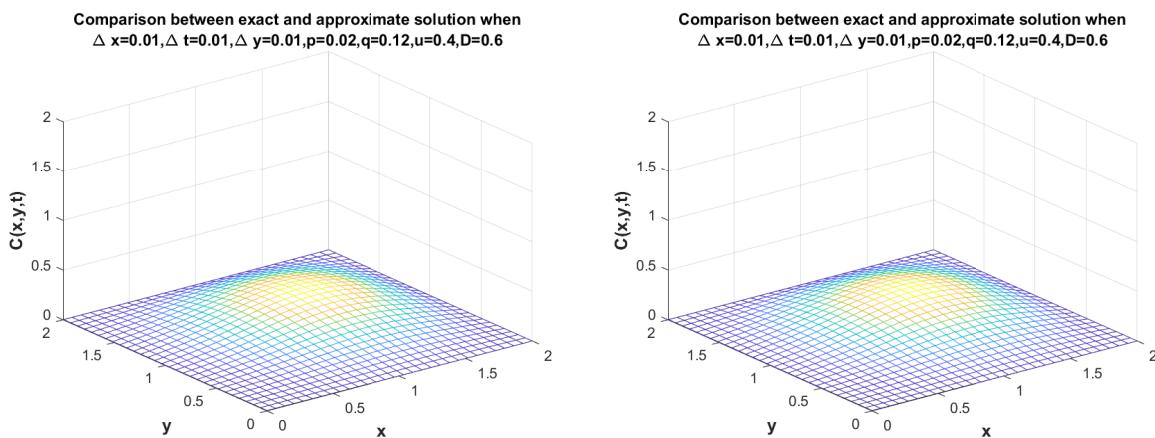


Figure 5. Comparison between exact and approximate solution for equation (9) with various values of D .

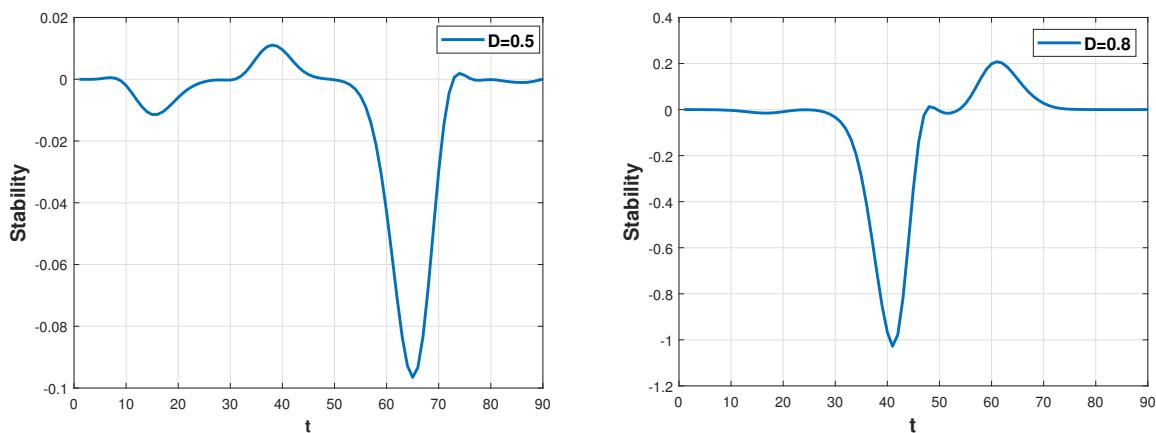


Figure 6. Stability of the approximate solution for equation (9) with various values of D .

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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