

Theta method comparative study of 2D asymmetric diffusion problem with convection on the wall

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Abstract: In this paper, numerical simulation based on generalized Crank-Nicolson method (which is also known as theta method) was performed in case of 2D diffusion problem with asymmetrical convection B.C on the walls. Also, model calibration was involved during numerical simulation model. Additionally, comparison between numerical and analytical solutions was made while qualitative compatibility was found between solutions. Moreover, maximum error between these solutions was found to be about 7.5%. Comparisons between other studies and current numerical and analytic solutions have been proved to be coincided.

Key-Words: Theta method, Diffusion, Crank-Nicolson, Analytical solution, Convection, Asymmetric B.C.

1 Introduction

Theta method which is also known as Crank-Nicolson (C-N) [1] generalized theory is defined as numerical weighted average scheme representation. This method is used in many fields, such as chemical and biological reactions and interactions [2-5], mechanics [6-12] and economics [13-15] applications. The mathematical behavior of the generalized formulation was studied by Nassif [16], Gurolay & Morris [17] and others [18-20]. In 1991, Stuart & Peplow [20] published their theoretical findings on dynamical equations system representation by numerical theta method. The existence of spurious asymptotic solutions which are not caused by numerical solution were obtained and compared to the current solution.

In this essay, theta method application will be demonstrated in case of 2D Diffusion equation with convection on the wall. Two-dimensional diffusion equation is derived using Fick's second law [19] and

its generalizations by Maxwell and others [20] who predict how diffusion causes the concentration to be varied over time. Numerical solutions for flowing fluid between two parallel plates without and with advection were obtained by Shariati *et al.* [21] and Appadu & Gidey [22]. A viscoelasticity fluid flow application with time-dependent parameter using theta method was studied by Chrispell *et al.* [23]. Moreover, temperature effect on transient free convection in MHD flow between two vertical parallel plates with variable mass diffusion was investigated by Rajput & Sahu [24]. In the latter study velocity profile and skin-friction were calculated and found. Convergence and stability of implicit methods for jump-diffusion systems were studied by Higham & Kloeden [25]. He was found that mean-square stability properties have been improved using implicit methods.

Convection at the boundary in case of temperature distribution was studied by Jordan Wall [26], Necati Özisik [27] and

Philippe Laval [28]. Also, numerical and analytical solution heat equation with derivative boundary conditions was studied by Cheniguel [29]. Comparisons between these studies and current study have been done and will be presented continuously.

The aim of this study is to solve two-dimensional steady state diffusion fluid problem with convective B.C. between two parallel plates using numerical and analytical solution development. Implicit, semi-implicit and explicit methods will be examined and compared by substituting different θ values. Moreover, comparison between analytical and numerical solutions will be presented and compared together with other studies.

2 Flow Field Equations

Consider a fluid with initial concentration c_0 which enters between two parallel plates with given distance L according to Fig. 1.

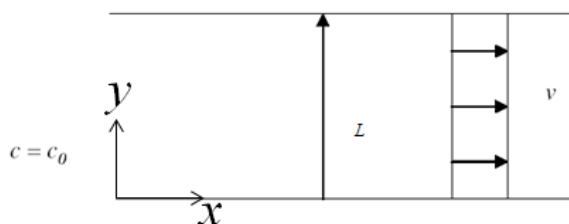


Fig. 1. 2D fluid diffusion model between two parallel plates.

It is assumed that mass transform occurs only by diffusion phenomena in the vertical direction along y-axis. Whilst in the horizontal direction (x-axis) mass transform is dominated mainly by convection phenomena. The 2D diffusion steady state parabolic equation is given by [29-31]:

$$\frac{\partial^2 C}{\partial Y^2} = \frac{\partial C}{\partial X}, \quad X > 0, \quad 0 \leq Y \leq L, \quad (1)$$

while $X = \frac{xD}{L^2v}$ and $Y = \frac{y}{L}$.

Where D represents diffusion constant, v is the flow velocity and L is the distance between the parallel plates.

Also, initial conditions are:

$$X = 0, \quad 0 \leq Y \leq L, \quad C = 1. \quad (2)$$

The convection conditions on the walls are:

$$\begin{cases} X > 0, \quad Y = L, \quad h_1 C + \frac{\partial C}{\partial Y} = 0 \\ X > 0, \quad Y = 0, \quad h_2 C - \frac{\partial C}{\partial Y} = 0 \end{cases}, \quad (3)$$

while $h_i = \frac{Lk_i}{D}$, $i = 1, 2, \dots$. Also, $h_1 = 0.1, 1, 10$

and $h_2 = 0.75h_1$.

Here, the problem has asymmetrical boundary conditions. Moreover, numerical calculation of $C(X, Y)$ should be performed until:

$$C(X, 0) = 0.05C_0, \quad C_0 = 1. \quad (4)$$

3 Numerical Methods Formulation

Numerical solution procedure for solving parabolic equation has been studied by [30-33]. Theta method formulation yields the following numerical algebraic equation:

$$\begin{aligned} \frac{C_{i,j+1} - C_{i,j}}{\delta_x} &= (1-\theta) \left(\frac{C_{i+1,j} - 2C_{i,j} + C_{i-1,j}}{\delta_y^2} \right) \\ &+ \theta \left(\frac{C_{i+1,j+1} - 2C_{i,j+1} + C_{i-1,j+1}}{\delta_y^2} \right) \end{aligned} \quad (5)$$

while $R = \frac{\delta_x}{\delta_y^2}$. Next, three methods which are derived from Eq. (5), will be discussed here.

Explicit method

Substituting $\theta = 0$ leads to the following explicit form:

$$\begin{aligned} \frac{C_{i,j+1} - C_{i,j}}{\delta_x} &= \frac{C_{i+1,j} - 2C_{i,j} + C_{i-1,j}}{\delta_y^2} \\ \rightarrow \end{aligned} \quad (6)$$

$$C_{i,j+1} = C_{i,j} + R(C_{i+1,j} - 2C_{i,j} + C_{i-1,j})$$

This method has conditioned stability according to:

$$\lambda = 1 - 2R(1 - \cos(\frac{\pi}{P})), |\lambda| \leq 1. \quad (7)$$

while $R \leq 0.5$.

C-N semi - implicit method

Substituting $\theta = 0.5$ leads to the following semi-implicit form:

$$C_{i,j+1} - C_{i,j} = \frac{R}{2} (C_{i+1,j} - 2C_{i,j} + C_{i-1,j} + C_{i+1,j+1} - 2C_{i,j+1} + C_{i-1,j+1})$$

$$\rightarrow 2(1+R)C_{i+1,j} - R(C_{i+1,j-1} - C_{i+1,j+1}) = 2(1-R)C_{i,j} + R(C_{i,j+1} + C_{i,j-1}) \quad (8)$$

while $i > 1, 3 \leq j \leq N - 1$. C-N method has unconditioned stability [29] for this kind of problem according to:

$$\lambda = \frac{1 - R(1 - \cos(\frac{\pi}{P}))}{1 + R(1 - \cos(\frac{\pi}{P}))}, |\lambda| \leq 1. \quad (9)$$

while $P \neq 0 \in \mathfrak{R}$.

Implicit method

Substituting $\theta = 1$ leads to the following implicit form:

$$\frac{C_{i,j+1} - C_{i,j}}{\delta_x} = \frac{C_{i+1,j+1} - 2C_{i,j+1} + C_{i-1,j+1}}{\delta_y^2}$$

$$\rightarrow C_{i,j+1} = C_{i,j} + R(C_{i+1,j+1} - 2C_{i,j+1} + C_{i-1,j+1}) \quad (10)$$

This method has unconditioned stability according to:

$$\lambda = \frac{1}{1 + 2R(1 - \cos(\frac{\pi}{P}))}, |\lambda| \leq 1. \quad (11)$$

Initial conditions numerical formulation is given by:

$$0 \leq Y \leq L, X = 0 : C(X, Y) = 1$$

$$C_{i_{jmean}} = 1, i_{jmean} = \frac{M}{2} \quad (12)$$

while $1 \leq i \leq M, 1 \leq j \leq N$. M will be determined by convergence condition $C(x, 0) \leq 0.05$. Boundary conditions

transpose numerical formulation $(X, Y) \rightarrow (i, j)$ yields:

$$Y = L, X > 0 : h_1 C + \frac{\partial C}{\partial Y} = 0 \rightarrow h_1 C = -\frac{\partial C}{\partial Y} \quad (13)$$

$$\rightarrow \frac{\partial C}{\partial Y} = \frac{C_{i,2} - C_{i,1}}{\Delta Y} \rightarrow C_{i,1} = \frac{C_{i,2}}{\Delta Y(\frac{1}{\Delta Y} - h_1)}$$

$$Y = 0, X > 0 : h_2 C - \frac{\partial C}{\partial Y} = 0$$

$$\rightarrow \frac{\partial C}{\partial Y} = \frac{C_{i,N} - C_{i,N-1}}{\Delta Y} \quad (14)$$

$$\rightarrow C_{i,N} = \frac{C_{i,N-1}}{\Delta Y(\frac{1}{\Delta Y} - h_2)}$$

while $i > 1$ and N is an arbitrary constant. Since C-N method has unconditioned stability and yields averaged values which are lined between the two other methods this method will be choose for solution. Moreover, R parameter has no influence on stability, but only on method accuracy.

Thomas Algorithm

In this section general formulation for solving numerical algebraic equation using Thomas algorithm will be introduced. Thomas tri-diagonal matrix is written by:

$$\begin{bmatrix} b_2 & c_2 & & & \\ a_3 & b_3 & c_3 & & \\ & a_4 & b_4 & c_4 & \\ & & \ddots & \ddots & \\ & & & a_{N-1} & b_{N-1} \end{bmatrix} \begin{bmatrix} C_{i,2} \\ C_{i,3} \\ \vdots \\ C_{i,N} \end{bmatrix} = \begin{bmatrix} d_2 \\ d_3 \\ \vdots \\ d_{N-1} \end{bmatrix} \quad (15)$$

From here, matrix parameters (15) will be calculated using Table 1, for each numerical method. In the next section analyzing of C-N numerical method results will be presented due to stability and averaged values magnitude as was explained in the previous section.

Table 1 Thomas algorithm parameters applications for theta method cases.

Parameters/Method	Explicit Method ($\theta = 0$)	C-N Method ($\theta = 0.5$)	Implicit Method ($\theta = 1$)
a_j	R	$-R$	$-R$
b_j	$1 - 2R$	$2(1 + R)$	$1 + 2R$
c_j	R	$-R$	$-R$
d_j	$C_{i-1,j+1}$	$R(C_{i-1,j+1}) + 2(1 - R)C_{i-1,j} + RC_{i-1,j-1}$	$C_{i-1,j}$
i, j	$i > 1, 3 \leq j \leq N - 1$ while $N \in \mathbb{N}$ is arbitrary		

4 Model Calibration

In this section C-N numerical method results will be examined. Flow concentration graphs for selected values of

$$R = \frac{\delta_x}{\delta_y^2}$$

near the wall ($Y = 0$) and in the middle section ($Y = 0.5$) are illustrated in Fig. 2.a-b. "Jumping" phenomenon of the fluid concentration occurs when h_1 parameter decreases with an increase in R parameter value. The current physical model cannot be applied when $R \gg h_1$. In other words, convection on the wall is found to be meaningless for specific R and h_1 ratios relative to other phenomenon which takes step in x direction. Therefore, one should use for example, general diffusion equation form which includes viscosity effect, or by considering other factors according to the specific problem.

Moreover, it seems that a difference between fluid concentration accuracy does exist between $Y = 0.5$ and $Y = 1$ sections. The smooth difference between walls concentration fluid is derived due to B.C. on the lower wall according to Eq. (3).

Examination of various convection parameter h_1 values in the context of fluid concentration on the wall ($Y = 0$) and in the middle section ($Y = 0.5$) is illustrated in Fig. 3.a-b. In similar way to the previous case, it seems that solution accuracy decreases with an increase in h_1 parameter value. Finally, it can be understood from comparison between Fig.2.a-b and Fig.3.a-b that fluid concentration is more sensitive to h_1 parameter than R parameter values. Next section discussion will be focused on specific numerical results.

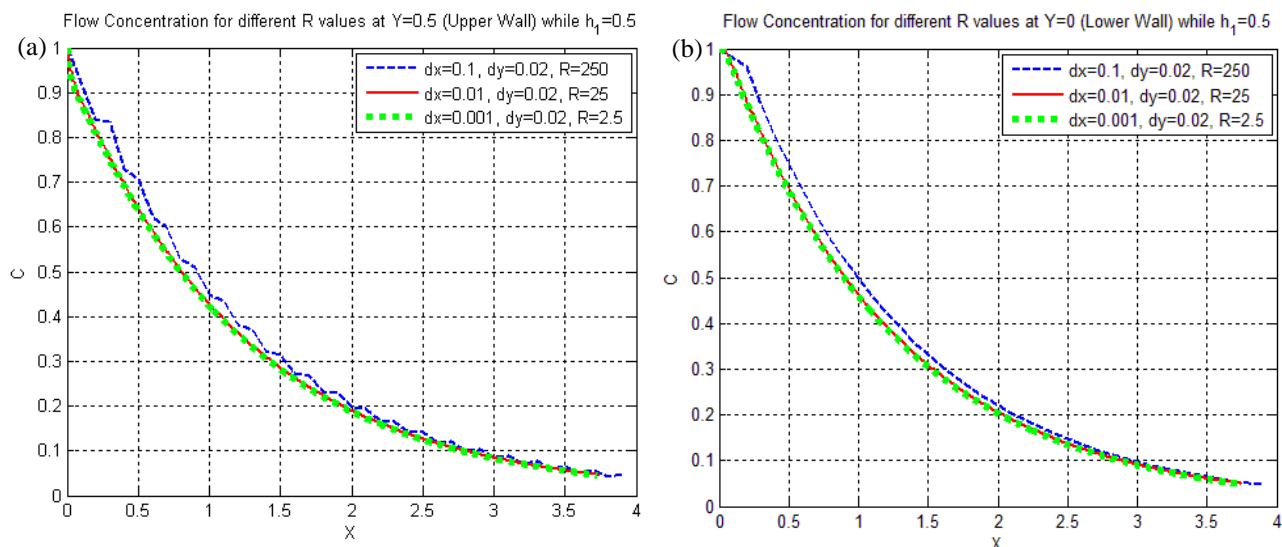


Fig. 2. Flow concentration for different R values at the: a. Middle section ($Y=0.5$). b. Lower wall ($Y=0$) while $h_1 = 0.5$.

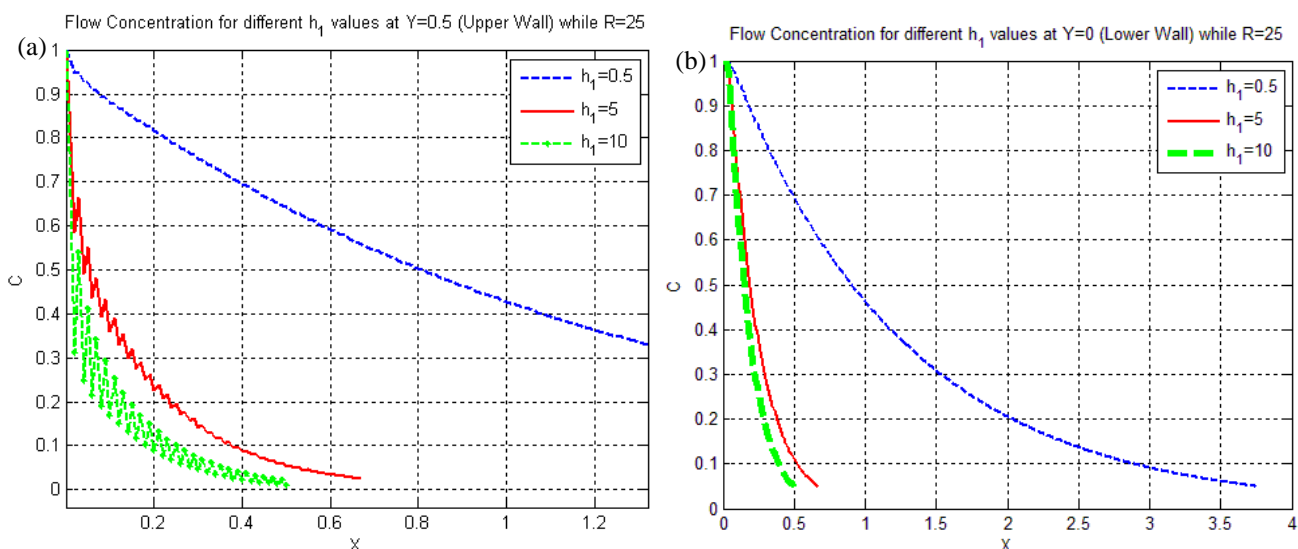


Fig. 3. Flow concentration for different h_1 values at the: a. Middle section ($Y=0.5$). b. Lower wall ($Y=0$) while $R = 25$.

5 Numerical Results

In this section numerical results will be presented for the following specific parameters:

- $\delta_x = 0.01, \delta_y = 0.02 \rightarrow R = 25$
and $h_1 = 0.05$.
- $\delta_x = 0.1, \delta_y = 0.02 \rightarrow R = 250$
and $h_1 = 0.01$.

On the one hand, it seems from Fig. 4.a-b that h, R parameters yield two different

quantitative results. On the other hand, qualitative solutions are similar in two-dimensional channel domain as shown in Fig.5.a-b. Flow concentration lines as shown in Fig. 6.a-b obtain their maximum and minimum values at $Y = 1$ and $Y = -1$, respectively. In the next section, analytical solution will be developed for results evaluation and comparative purposes.

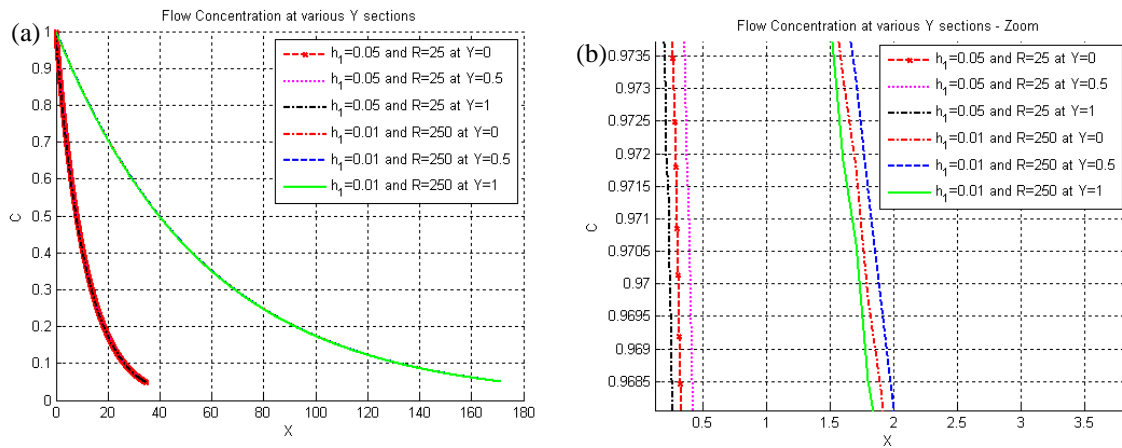


Fig. 4. Flow concentration for different h_1, R values at the: Middle section ($Y=0.5$), Upper ($Y=1$) and Lower wall ($Y=0$) while $R = 25, 250$.

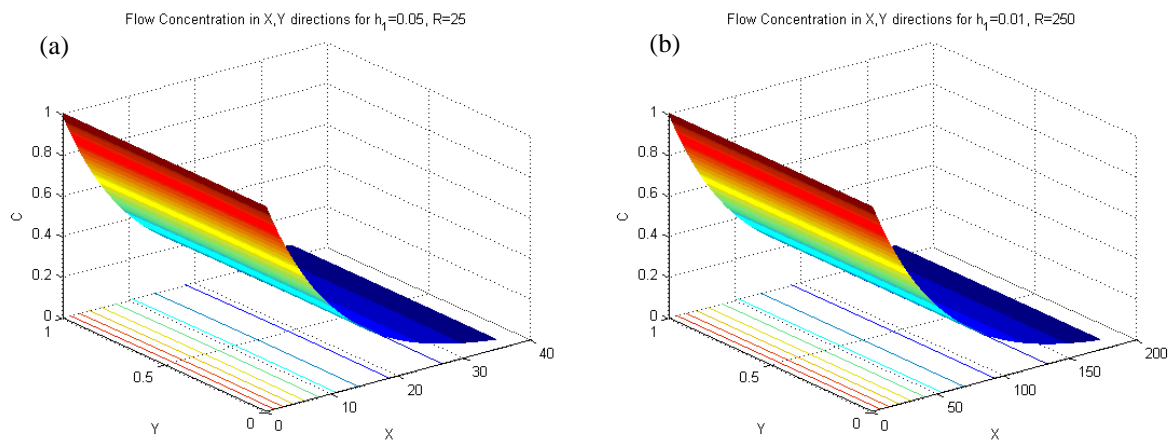


Fig. 5. Flow concentration in X-Y directions for different h_1, R values: a. $h_1 = 0.05, R = 25$. b. $h_1 = 0.01, R = 250$.

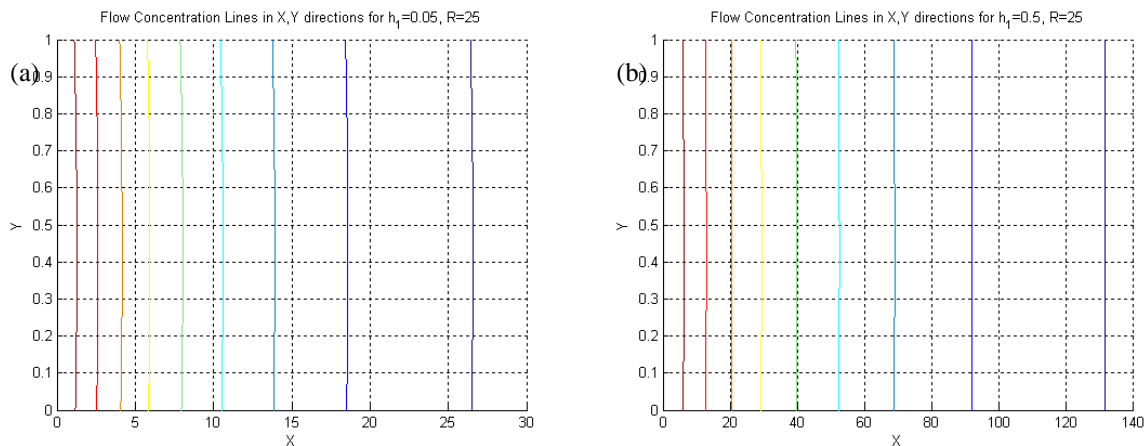


Fig. 6. Flow concentration lines in X-Y directions for different h_1, R values: a. $h_1 = 0.05, R = 25$. b. $h_1 = 0.01, R = 250$.

6 Analytical Solution

The mathematical formulation of the problem is to find concentration function $C(X, Y)$ such that:

$$\frac{\partial^2 C}{\partial Y^2} = \frac{\partial C}{\partial X}, \quad X > 0, \quad 0 \leq Y \leq L, \quad (16)$$

With convective B.C. on the wall as follows:

$$\begin{cases} h_1 C(X, L) + \frac{\partial C}{\partial Y}(X, L) = 0 \\ h_2 C(X, 0) - \frac{\partial C}{\partial Y}(X, 0) = 0 \end{cases} \quad (17)$$

while $X > 0$. Initially, the concentration fulfills:

$$C(0, Y) = 1, \quad 0 \leq Y \leq L. \quad (18)$$

Now, analytical solution will be performed using separate variable procedure according to Necati Özisik and Wall notes [26-27]. Assume that solution has the following form:

$$C(X, Y) = U(X)T(Y). \quad (19)$$

Substituting (19) into (16) leads to:

$$\frac{1}{T} \frac{\partial^2 T}{\partial Y^2} = \frac{1}{U} \frac{\partial U}{\partial X} = -\lambda^2. \quad (20)$$

Hence, the solution for $U(X)$ is:

$$U(X) = a_1 e^{-\lambda^2 X}, \quad a_1 = C_0 = 1. \quad (21)$$

while a_1 is constant and $T(Y)$ is the solution of the following eigenvalue problem:

$$T'' + \lambda^2 T = 0, \quad (22)$$

Where homogenous solution is given by:

$$T = a_2 \cos(\lambda Y) + a_3 \sin(\lambda Y), \quad (23)$$

while a_2, a_3 are constants and $\lambda > 0$ (if $\lambda < 0$ then problem is diverged).

In order to find a_2, a_3 B.C. (17) will be written such as:

$$\begin{cases} a_2 \cos(\lambda L) + a_3 \sin(\lambda L) = -\frac{\lambda}{h_1} [a_3 \cos(\lambda L) - a_2 \sin(\lambda L)] \\ a_2 = \frac{\lambda}{h_2} a_3 \end{cases} \quad (24)$$

From here, we get the following relation:

$$\frac{\lambda}{h_2} \left[\cos(\lambda L) - \frac{\lambda}{h_1} \sin(\lambda L) \right] + \left[\sin(\lambda L) + \frac{\lambda}{h_1} \cos(\lambda L) \right] = 0$$

→

$$\tan(\lambda L) = \frac{\lambda(h_1 + h_2)}{\lambda^2 - h_1 h_2}$$

→

$$h_2 = 0.75 h_1, L = 1$$

$$\tan(\lambda) = \frac{1.75 h_1}{\lambda^2 - 0.75 h_1^2} \lambda$$

(25)

Where $T(Y)$ form will be given by:

$$T(Y) = a_3 \left[\frac{\lambda}{h_2} \cos(\lambda Y) + \sin(\lambda Y) \right]. \quad (26)$$

Therefore, the complete solution is of the form:

$$C(X, Y) = \sum_{m=1}^{\infty} a_m \left[\frac{\lambda}{h_2} \cos(\lambda Y) + \sin(\lambda Y) \right] e^{-\lambda^2 X} \quad (27)$$

The specific eigenfunctions are obtained by incorporating the initial conditions:

$$f(Y) = 1 = \sum_{m=1}^{\infty} a_m \left[\frac{\lambda}{h_2} \cos(\lambda Y) + \sin(\lambda Y) \right], \quad (28)$$

which expresses the representation of $f(Y)$ in terms of eigenfunctions and requires that:

$$a_m = \frac{\int_0^L \frac{\lambda}{h_2} \cos(\lambda Y) + \sin(\lambda Y) dY}{\int_0^L \left[\frac{\lambda}{h_2} \cos(\lambda Y) + \sin(\lambda Y) \right]^2 dY} = \frac{\frac{\sin(\lambda L)}{h_2} + \frac{1 - \cos(\lambda L)}{\lambda}}{\frac{\sin(2\lambda L)}{4\lambda} \left[\left(\frac{\lambda}{h_2} \right)^2 - 1 \right] + \frac{1 - \cos(2\lambda L)}{2h_2} + \frac{L}{2} \left[1 + \left(\frac{\lambda}{h_2} \right)^2 \right]} \quad (29)$$

7 Comparison & Discussion

In this section comparison between numerical solution and analytical solution will be presented and discussed. Qualitative compatibility between analytic and

approximate solutions was found as shown in Fig. 7. a. Maximum error value between solutions is about 7.5% as calculated using Fig. 7. b. The main reasons for this difference are derived from:

- Numerical solution convergence condition (4) – "Stop Condition".
- Number of members in series eq. (27).
- Numerical solution discretization.

Moreover, it seems that both solutions have similar qualitative behavior as shown in Fig. 7-9.

Analogous behavior between concentration and temperature difference does exist. Therefore, comparisons to heat and mass transfer studies will be performed. Analytical and numerical solutions are coincided with Khan and Gorla results [34] (see Fig. 9. a from Ref. [34] compared to Fig. 7 in the current article). The graph in Fig. 10.a predicts different nano-fluids temperature behavior over a non-isothermal stretching wall with convective boundary condition. Another study deals with 2D heat

transfer problem including mixed boundary conditions was studied by Chaabane *et al* [35]. This problem was solved numerically using Lattice Boltzmann simulations method. It can be observed from Fig. 10.b that solution qualitative behavior and order of magnitude are similar to current study results as compared to Fig. 7. Sakimoto and Zuber have investigated convective cooling phenomenon in lava tubes. Their study explains the wide range of implied cooling rates by considering forced convection as a dominant cooling process in lava tubes. Fig. 11 relates to mean temperature distribution versus the distance from the vent through steady laminar flow between parallel plates with constants temperature and material properties. Correspondence between latter study results and current study does exist in the qualitative and quantitative (order of magnitude) aspects (compare Fig. 11 to Fig. 7).

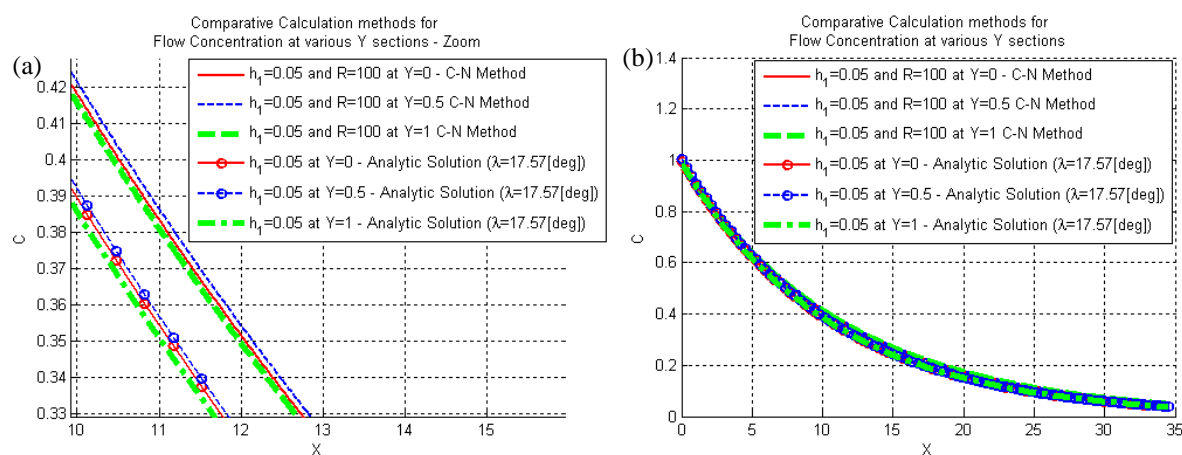
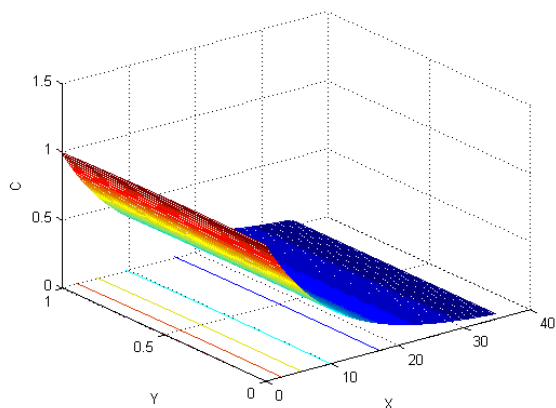


Fig. 7. Comparative calculation methods for flow concentration at various Y sections.

(a) Analytic solution for Flow Concentration in X,Y directions where $h_1=0.01$



(b) Numerical solution for Flow Concentration in X,Y directions where $h_1=0.01$ and $R=100$

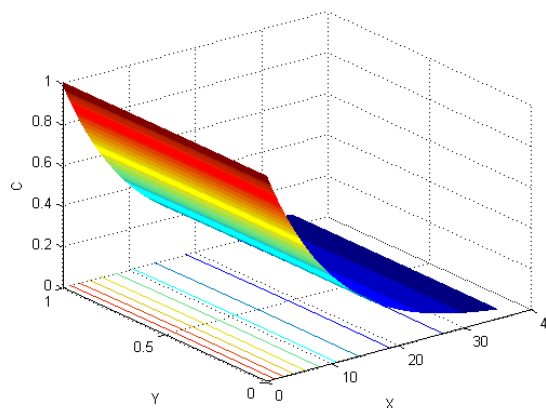
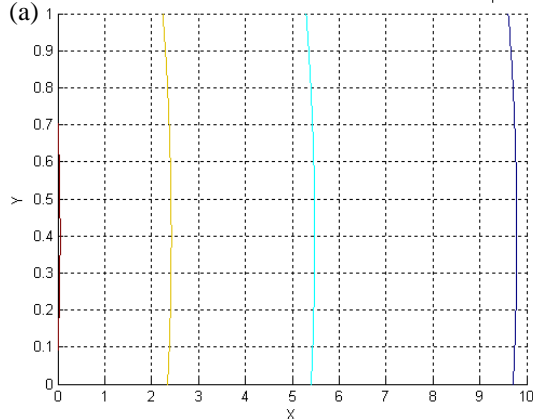


Fig. 8. Comparative calculation methods for X – Y directions: a. Analytical solution for flow concentration. b. Numerical solution for flow concentration.

(a) Analytic solution for Flow Concentration lines in X,Y directions where $h_1=0.01$



(b) Numerical solution for Flow Concentration lines in X,Y directions where $h_1=0.01$ and $R=100$

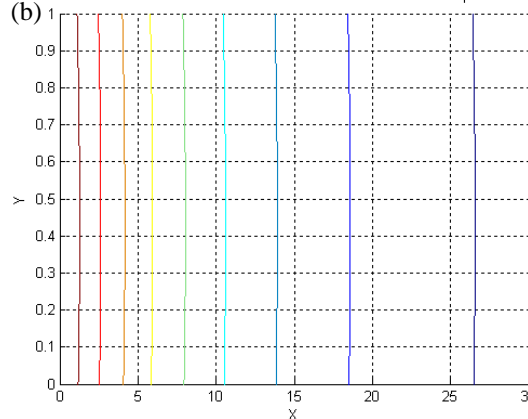


Fig. 9. Comparative calculation methods for X – Y directions: a. Analytic solution for Flow Concentration lines. b. Numerical solution for Flow Concentration lines.

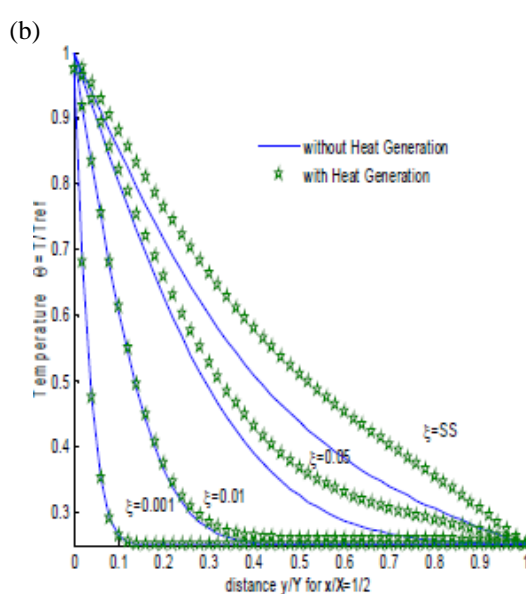
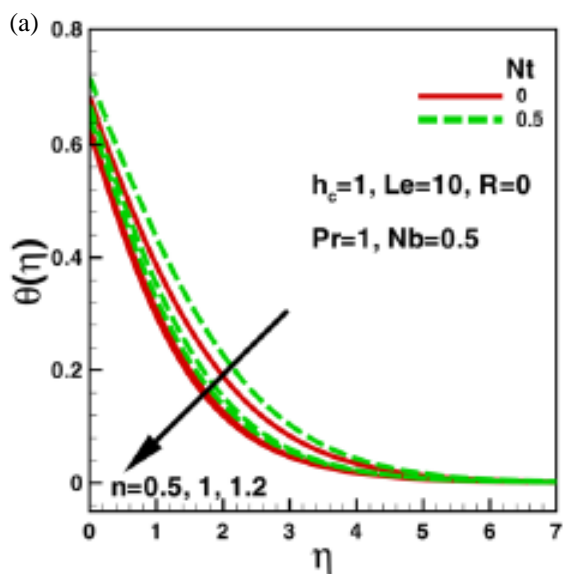


Fig. 10. a. Effect of generalized Prandtl number Pr and thermophoresis parameter on dimensionless temperature for different non-Newtonian nanofluids by Khan and Gorla [34]. b. Comparison of

centreline ($x/X=0.5$) temperature in the presence and the absence of heat generation by R. Chaabane *et al* [35].

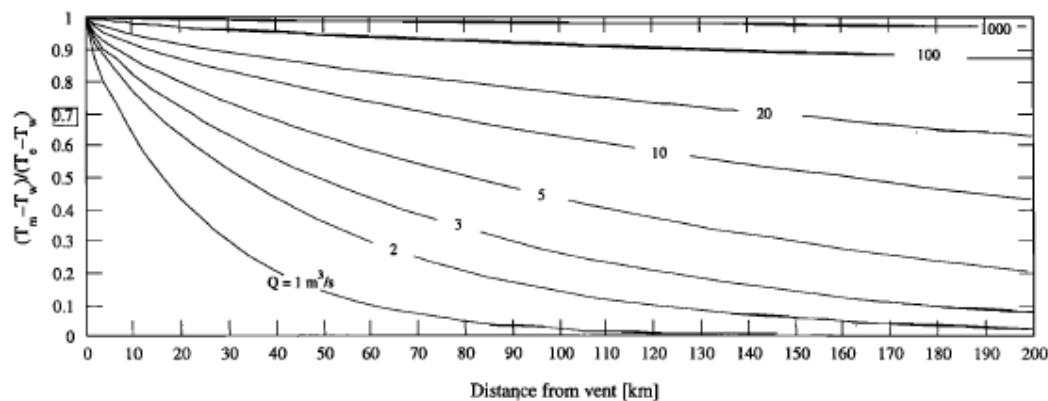


Fig. 11. Temperatures predicted for parallel plate flow with a height: width ratio of 1:5, an entrance temperature of 1160°C , and a wall temperature of 1077°C by Sakimoto and Zuber [36].

8 Conclusion

This study presents numerical simulation of 2D diffusion problem with asymmetrical convection on the walls based on generalized Crank-Nicolson method and Thomas algorithm. In order to estimate numerical parameter influences, model calibration was performed during numerical simulation model. It was found

that $R = \frac{\delta_x}{\delta_y^2}$ and h_1 parameters have great

influence on solution accuracy only. The current physical model cannot be applied when $R \gg h_1$. Taking it in account, one should use general diffusion equation form including viscosity effect. It seems that solution accuracy is decreasing with h_1 increasing value. Also, it was found that fluid concentration absolute value is more sensitive to h_1 parameter than R parameter values. Flow concentration results obtained their maximum and minimum values at $Y = 1$ and $Y = -1$, respectively. Comparison between numerical and analytical solution was made while qualitative compatibility was found between solutions. Moreover, maximum error between these solutions was found to be about 7.5%. Comparisons between other studies [34-36] on heat and mass transfer field and current numerical and analytical solution have been proved to be coincided.

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