Numerical solution to Diffusion of Chemically Reactive Species of a Casson Fluid Flow over an Exponentially Stretching Surface

T.Hymavathi[1]* and W.Sridhar[2]

Department of Mathematics, Adikavi Nannaya University, Rajamundry, India
*Corresponding Author

Abstract

The present study of the paper deals with diffusion of chemically reactive species of a non-Newtonian fluid towards an exponentially stretching surface using keller box method. Casson fluid model is used to characterize the non-Newtonian fluid behaviour. The flow fields and mass transfer are affected significantly by the physical parameters. The effect of increasing values of the Casson parameter is to suppress the velocity field. But the concentration increases with increase in Casson parameter.

Keywords: Casson fluid, exponentially stretching sheet, chemical reaction

I. INTRODUCTION

Boundary layer flow over a stretching surface is often encountered in many engineering disciplines. The study of boundary layer flow over a linearly stretching surface in most of the available literature. The flow due to nonlinearly stretching sheet by considering exponential order stretching velocity is available in literature.

In the present investigation, non-Newtonian fluid model known as Casson fluid model is considered. For a Casson fluid, if a shear stress less than the yield stress is applied to the fluid, it behaves like a solid whereas if a shear stress greater than yield stress is applied, it starts to move. Some examples of Casson fluid are human blood, concentrated fruit juices, Jelly, tomato sauce, honey, soup etc. Casson fluid can be defined as a shear thinning liquid which is assumed to have an infinite viscosity at zero rate of shear, a yield stress below which no flow occurs and a zero viscosity at an
infinite rate of shear (Dash et al. [6]). Eldabe and Elmohands [7] have studied the Casson fluid for the flow between two rotating cylinders and Boyd et al. [8] investigated the Casson fluid flow for the steady and oscillatory blood flow. Swati mukhopadhyay et al [5] analyzed the diffusion of chemically reactive species of a Casson fluid flow over an exponentially stretching surface using RK method. Recently, Hymavathi et al [10] studied the numerical solution to mass transfer on MHD flow of Casson fluid with suction and chemical reaction.

The purpose of this present work is to study the flow and mass transfer analysis in boundary layer flow of a Casson fluid over an exponentially stretching sheet in presence of a first order constructive/destructive chemical reaction numerically using keller box method. Using similarity transformations, a third order ordinary differential equation corresponding to the momentum equation and a second order differential equation corresponding to the concentration equation are derived. Numerical calculations up to desired level of accuracy were carried out for different values of dimensionless parameters of the problem under consideration for the purpose of illustrating the results graphically. The analysis of the results shows that the flow field is influenced appreciably by the mass transfer parameter in presence of constructive, non-reactive and destructive chemical reactions.

II. EQUATIONS OF MOTION

Let us consider the flow of an incompressible viscous fluid past a flat sheet coinciding with the plane \( y = 0 \). The fluid flow is confined to \( y > 0 \). Two equal and opposite forces are applied along the \( x \)-axis so that the wall is stretched keeping the origin fixed (Fig.1). The rheological equation of state for an isotropic and incompressible flow of a Casson fluid is

\[
\tau_j = \begin{cases} 
2(\mu_B + \frac{p_y}{\sqrt{2\pi}})e_{ij}, \pi > \pi_c \\
2(\mu_B + \frac{p_y}{\sqrt{2\pi_c}})e_{ij}, \pi < \pi_c 
\end{cases}
\]

Here \( \pi = e_{ij}e_{ij} \) and \( e_{ij} \) is the (i,j)-th component of the deformation rate, \( \pi \) is the product of the component of deformation rate with itself, \( \pi_c \) is a critical value of this product based on the non-Newtonian model, \( \mu_B \) is plastic dynamic viscosity of the non-Newtonian fluid, and \( p_y \) is the yield stress of the fluid. Let \( C_w \) be the concentration at the sheet and concentration far away from the sheet is \( C_\infty \). Also the reaction of species is the first order homogeneous chemical reaction with rate constant \( k \).
The continuity, momentum (Mustafa et al. [3]) and concentration equations governing such type of flow are written as

\[
\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} = 0
\]  

(1)

\[
u \frac{\partial u}{\partial x} + v \frac{\partial u}{\partial y} = \nu \left(1 + \frac{1}{\beta}\right) \frac{\partial^2 u}{\partial y^2}
\]  

(2)

\[
u \frac{\partial C}{\partial x} + v \frac{\partial C}{\partial y} = D \frac{\partial^2 C}{\partial y^2} - k(C - C_\infty)
\]  

(3)

where \(u \) and \(v \) are the components of velocity respectively in the \(x \) and \(y \) directions, \(\nu \) is the kinematic viscosity, \(\rho \) is the fluid density (assumed constant), \(\beta = \frac{\mu_B \sqrt{2\pi c}}{2P_y} \) is parameter of the Casson fluid, \(D \) is the diffusion coefficient of the diffusing species in the fluid, \(k = k_0 e^{\frac{z}{L}} \) is the exponential reaction rate; \(k>0 \) stands for destructive reaction whereas \(k<0 \) stands for constructive reaction, \(k_0 \) is a constant.

A. Boundary Conditions

The appropriate boundary conditions for the problem are given by

\(u \) at \( y = 0, u = U, v = 0, C \rightarrow C_w \)

as \( y \rightarrow \infty, v \rightarrow 0, C \rightarrow C_\infty \)  

(4)

Here \( U = U_0 e^{\frac{x}{L}} \) is the stretching velocity (Magyari and Keller [2]), \( C_w = C_\infty + C_0 e^{\frac{x}{P_y}} \) is the concentration at the sheet, \(U_0, C_0\) are the reference velocity, concentration respectively.

B. Method of solution
Introducing the similarity variables as

\[ \eta = \frac{\bar{u}_0}{2\nu L} e^{\frac{x}{2L}} \]

\[ u = U_0 e^{\frac{x}{L}} f'(\eta) \]

\[ v = -\frac{\nu \bar{u}_0}{2L} e^{\frac{x}{2L}} \{ f(\eta) + \eta f'(\eta) \} \]

\[ C = C_\infty e^{\frac{x}{2L}} \phi(\eta) \]  \hspace{1cm} (5)

and upon substitution of (5) in equations (2) and (3) the governing equations reduce to

\[ \left( 1 + \frac{1}{\beta} \right) f'''' + f f''' - 2 f'^2 = 0 \]

\[ \phi'' - Sc (f \phi' - f' \phi - 2 \gamma \phi) = 0 \]  \hspace{1cm} (6)

and the boundary conditions take the following form

at \( \eta = 0, f = 0, \phi = 1, f' = 1 as \eta \to \infty, f' \to 0, \phi \to 0 \)

where the prime denotes differentiation with respect to \( \eta \),

\[ Sc = \frac{v}{D} \]  \hspace{1cm} is the Schmidt number, \( \gamma = \frac{k_0}{u_0} \)  \hspace{1cm} is the reaction rate parameter. Here \( \gamma > 0 \) represents the destructive reaction, \( \gamma = 0 \) corresponds to no reaction, and \( \gamma < 0 \) stands for the generative reaction.

**Numerical Procedure**

Equation subject to boundary conditions is solved numerically using an implicit-finite difference scheme known as keller box method, as described by cebeci and Bradshaw\(^9\). The steps followed are

1. Reduce (1) to a first order equation
2. Write the difference equations using central differences
3. Linearize the resulting algebraic equation by Newton’s method and write in matrix vector form
4. Use the block tridiagonal elimination technique to solve the linear system.

Consider the flow equation and concentration equation

\[ \left( 1 + \frac{1}{\beta} \right) f'''' + f f''' - 2 f'^2 = 0 \]

\[ \phi'' - Sc (f \phi' - f' \phi - 2 \gamma \phi) = 0 \]

and the boundary conditions
Numerical solution to Diffusion of Chemically Reactive Species of a Casson...

\[ f(\eta) = 0, f'(\eta) = 1, \phi(\eta) = 1 \text{ at } \eta = 0 \]
\[ f'(\eta) \to 0, \phi(\eta) \to 0 \text{ at } \eta \to \infty \]

Introduce \( f' = p \), \( g' = n \) \hfill (7) \hfill (8) \hfill (9)

Eqn (5) reduces to
\[ \left( 1 \frac{1}{\beta_J} \right) q' + f q - 2 p^2 = 0 \] \hfill (10)
\[ n' + Sc(f n - p g - 2 \gamma g) = 0 \] \hfill (12)

Consider the segment \( \eta_{j-1}, \eta_j \) with \( \eta_{j-1/2} \) as the mid point
\[ \eta^0 = 0, \eta_j = \eta_{j-1} + h_j, \eta_J = \eta_{\infty} \] \hfill (13)

where \( h_j \) is the \( \Delta \eta \) spaces and \( j=1,2,\ldots,J \) is a sequence number that indicates the coordinate locations.

\[ \frac{f_j - f_{j-1}}{h_j} = \frac{p_j + p_{j-1}}{2} = p_{j-1/2} \] \hfill (14)
\[ \frac{p_j - p_{j-1}}{h_j} = \frac{q_j + q_{j-1}}{2} = q_{j-1/2} \] \hfill (15)
\[ \frac{g_j - g_{j-1}}{h_j} = \frac{n_j + n_{j-1}}{2} = n_{j-1/2} \] \hfill (16)
\[ q_j - q_{j-1} + \frac{\beta h_j}{\beta + 1} \left( \frac{f_j + f_{j-1}}{2} \right) \left( \frac{q_j + q_{j-1}}{2} \right) - 
\frac{2 \beta h_j}{(\beta + 1)} \left( \frac{p_j + p_{j-1}}{2} \right)^2 \] \hfill (18)

Equations (14) to (18) are imposed for \( j=1,2,3,\ldots,J \) and the transformed boundary layer thickness \( \eta_j \) taken to the sufficiently large so that it is beyond the edge of the boundary layer.

The bc’s are \( f_0 = 0, p_1 = 0 \) \hfill (19)
\[ p_0 = 1, g_0 = 1, g_J = 0 \]

Newton’s method
Linearizing the non linear system of equations (14) to (18)

Introduce

\[ f_j^{(k+1)} = f_j^{(k)} + \delta f_j \]

\[ p_j^{(k+1)} = p_j^{(k)} + \delta p_j \]

\[ q_j^{(k+1)} = q_j^{(k)} + \delta q_j \]

\[ g_j^{(k+1)} = g_j^{(k)} + \delta g_j \]

\[ n_j^{(k+1)} = n_j^{(k)} + \delta n_j \]  \hspace{1cm} (20)

Substitute in equations (14) to (18)

\[ \delta f_j - \delta f_{j-1} - \frac{h_j}{2} (\delta p_j + \delta p_{j-1}) = (r_1)_{j-\frac{1}{2}} \]  \hspace{1cm} (21)

\[ \delta p_j - \delta p_{j-1} - \frac{h_j}{2} (\delta q_j + \delta q_{j-1}) = (r_2)_{j-\frac{1}{2}} \]  \hspace{1cm} (22)

\[ \delta g_j - \delta g_{j-1} - \frac{h_j}{2} (\delta n_j + \delta n_{j-1}) = (r_3)_{j-\frac{1}{2}} \]  \hspace{1cm} (23)

\[ (a_1)_{j} \delta f_j + (a_2)_{j} \delta f_{j-1} + (a_1)_{j} \delta f_j + (a_2)_{j} \delta f_{j-1} + (a_3)_{j} \delta f_j + (a_4)_{j} \delta f_{j-1} + (a_5)_{j} \delta f_j + (a_6)_{j} \delta f_{j-1} = (r_4)_{j-\frac{1}{2}} \]  \hspace{1cm} (24)

\[ (b_1)_{j} \delta n_j + (b_2)_{j} \delta n_{j-1} + (b_1)_{j} \delta n_j + (b_2)_{j} \delta n_{j-1} + (b_3)_{j} \delta n_j + (b_4)_{j} \delta n_{j-1} + (b_5)_{j} \delta n_j + (b_6)_{j} \delta n_{j-1} = (r_5)_{j-\frac{1}{2}} \]  \hspace{1cm} (25)

Where
\[
t_j - t_{j-1} + \text{Sch}_j \left( \frac{f_j + f_{j-1}}{2} \right) \left( \frac{t_j + t_{j-1}}{2} \right) - \text{Sch}_j \left( \frac{p_j + p_{j-1}}{2} \right) \left( \frac{g_j + g_{j-1}}{2} \right) - \text{Sc}\gamma h_j \left( \frac{g_j + g_{j-1}}{2} \right) = 0
\]

\[
(a_1)_j = 1 + \frac{\beta h_j}{4(\beta + 1)}(f_j + f_{j-1})
\]

\[
(a_2)_j = (a_1)_j - 2.0
\]

\[
(a_3)_j = \frac{\beta h_j}{4(\beta + 1)}(q_j + q_{j-1})
\]

\[
(a_4)_j = (a_3)_j
\]

\[
(a_5)_j = \frac{\beta h_j}{(\beta + 1)}(p_j + p_{j-1})
\]

\[
(a_6)_j = (a_5)_j
\]

\[
(b_1)_j = 1 + \frac{\text{Sch}_j}{4}(f_j + f_{j-1})
\]

\[
(b_2)_j = (b_1)_j - 2.0
\]

\[
(b_3)_j = \frac{\text{Sch}_j}{4}(n_j + n_{j-1})
\]

\[
(b_4)_j = (b_3)_j
\]

\[
(b_5)_j = -\frac{\text{Sch}_j}{4}(g_j + g_{j-1})
\]

\[
(b_6)_j = (b_5)_j
\]

\[
(b_7)_j = -\frac{\text{Sch}_j}{4}(p_j + p_{j-1}) - \text{Sc}\gamma h_j
\]

\[
(b_8)_j = (b_7)_j
\]

And
\[(r_1)_j = f_{j-1} - f_j + \frac{h_j}{2}(p_j + p_{j-1}) \]
\[(r_2)_j = p_{j-1} - p_j + \frac{h_j}{2}(q_j + q_{j-1}) \]
\[(r_3)_j = g_{j-1} - g_j + \frac{h_j}{2}(n_j + n_{j-1}) \]
\[(r_4)_j = q_{j-1} - q_j - \frac{β_j}{4(β+1)}(f_j + f_{j-1})(g_j + q_{j-1}) + \frac{β_j}{2(β+1)}(p_j + p_{j-1}) \]
\[(r_5)_j = n_{j-1} - n_j - \frac{Sch_j}{4}(f_j + f_{j-1})(n_j + n_{j-1}) + \frac{Sch_j}{4}(p_j + p_{j-1})(g_j + g_{j-1}) + Sc_\gamma h_j(g_j + g_{j-1}) \]  

Taking \( j=1,2,3,\ldots \)

The system of equations becomes

\[ [A_1][\delta_1]+[C_1][\delta_2]=[r_1] \]  
\[ [B_2][\delta_1]+[A_2][\delta_2]+[C_2][\delta_3] = [r_2] \]  
\[ \ldots [B_{1-1}][\delta_1]+[A_{1-1}][\delta_2]+[C_{1-1}][\delta_3] = [r_{1-1}] \]  
\[ [B_1][\delta_{1-1}]+[A_1][\delta_1] = [r_1] \]

Where

\[ A_i = \begin{bmatrix} 0 & 0 & 1 & 0 & 0 \\ d & 0 & 0 & d & 0 \\ 0 & d & 0 & 0 & d \\ (a_{2})_1 & 0 & (a_{3})_1 & 0 & (a_{1})_1 \\ 0 & (b_{2})_1 & (b_{3})_1 & 0 & (b_{1})_1 \end{bmatrix} \]
\[ A_j = \begin{bmatrix} d & 0 & 1 & 0 & 0 \\ -1 & 0 & 0 & d & 0 \\ 0 & -1 & 0 & 0 & d \\ (a_{6})_j & 0 & (a_{5})_j & 0 & (a_{4})_j \\ (b_{6})_j & (b_{5})_j & (b_{4})_j & 0 & (b_{3})_j \end{bmatrix} \]

\[ B_j = \begin{bmatrix} 0 & 0 & -1 & 0 & 0 \\ 0 & 0 & 0 & d & 0 \\ 0 & 0 & 0 & 0 & d \\ 0 & 0 & (a_{4})_j & (a_{3})_j & 0 \\ 0 & 0 & (b_{4})_j & 0 & (b_{2})_j \end{bmatrix} \]
\[ C_j = \begin{bmatrix} d & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 \\ (a_{5})_j & 0 & 0 & 0 & 0 \\ (b_{5})_j & (b_{4})_j & 0 & 0 & 0 \end{bmatrix} \]
The Block Elimination Method

The linearized differential equations of the system has a block diagonal structure. This can be written in matrix form as

\[
\begin{pmatrix}
A_1 & C_1 & \cdots & \cdots \\
B_2 & A_2 & & \\
\vdots & \ddots & \ddots & \\
B_{j-1} & A_{j-1} & C_{j-1} & \cdots \\
B_j & A_j & C_j & \cdots \\
\end{pmatrix} \begin{pmatrix}
[\alpha_1] \\
[\beta_2] \\
\vdots \\
[\beta_{j-1}] \\
[\beta_j] \\
\end{pmatrix} = \begin{pmatrix}
[\delta_1] \\
[\delta_2] \\
\vdots \\
[\delta_{j-1}] \\
[\delta_j] \\
\end{pmatrix} = \begin{pmatrix}
[r_1] \\
[r_2] \\
\vdots \\
[r_{j-1}] \\
[r_j] \\
\end{pmatrix}
\]

This is of the form \( A \delta = r \) \hspace{1cm} (31)

To solve the above system

Write \( [A] = [L] [U] \) \hspace{1cm} (32)

Where

\[
L = \begin{pmatrix}
[\alpha_1] & & & & \\
[\beta_2] & [\alpha_2] & & & \\
& \ddots & \ddots & \ddots & & \\
& & [\beta_{j-1}] & [\alpha_{j-1}] & & \\
& & & \beta_j & [\alpha_j] & \\
\end{pmatrix}
\]

and

\[
U = \begin{pmatrix}
[I] & [\Gamma_1] & & & & \\
[I] & [\Gamma_2] & & & & \\
& \ddots & \ddots & \ddots & \ddots & \\
& & [I] & [\Gamma_{j-1}] & & \\
& & & [I] & [\Gamma_j] & \\
\end{pmatrix}
\]

Where \([I]\) is the identity matrix

\([\alpha_i], [\Gamma_i]\) are determined by the following equations

\[ [\alpha_i] = [A_i] \]
\[ [A_i][\alpha_i] = [C_i] \]
\[ [\alpha_j] = [A_j] - [B_j][\Gamma_{j-1}] \hspace{1cm} j=2,3, \ldots, J \]
\[ [\alpha_j][\Gamma_j] = [C_j] \hspace{1cm} j=2,3, \ldots, J-1 \]

Substituting (33) in (32)

\[ LU\delta = r \]

Let \( U \delta = W \)

then \( LW = r \)
where \( W = \begin{bmatrix} w_1 \\ w_2 \\ w_{j-1} \\ w_j \end{bmatrix} \)

Now \( \alpha_j \begin{bmatrix} w_1 \\ w_2 \end{bmatrix} = \begin{bmatrix} r_1 \end{bmatrix} \)

\( \alpha_j \begin{bmatrix} w_1 \\ w_2 \end{bmatrix} = \begin{bmatrix} r_1 \end{bmatrix} - \begin{bmatrix} B_j \end{bmatrix} \begin{bmatrix} W_{j-1} \end{bmatrix} \) for \( 2 \leq j \leq J \)

Once the elements of \( W \) are found, substitute in \( L\delta = W \) and solve for \( \delta \)

\( \delta_j = \begin{bmatrix} W_j \end{bmatrix} \)

\( \delta_j = \begin{bmatrix} W_j \end{bmatrix} - \begin{bmatrix} \Gamma_j \end{bmatrix} [\delta_{j+1}] \), \( 1 \leq j \leq J-1 \)

These calculations are repeated until some convergence criterion is satisfied and we stop the calculations when \( |\delta g_0^{(i)}| \leq \varepsilon \), where \( \varepsilon \) is very small prescribed value taken to be \( \varepsilon = 0.0000001 \).

### III. RESULTS AND DISCUSSIONS

In order to analyze the results, numerical computations have been carried out using the method described in the previous section for various values of Casson parameter (\( \beta \)), Schmidt number (\( Sc \)) and reaction rate parameter (\( \gamma \))

![Fig 1a: Velocity profiles for various values of casson parameter](image)

Figure 1a shows that the effect of casson parameter on velocity profiles. Considering
γ=0.3, Sc=10 and Casson parameter β at 0.5, 1.0 and 1.5, it is observed that velocity is found to decrease with the increase in Casson parameter β.

**Fig 1b:** Velocity profiles for various values of scadmith number Sc

Figure 1b shows that the effect of casson parameter on velocity profiles. Considering γ=1.0, β=1.0 and scadmith number Sc at 0.5, 1.0 and 2.0, it is observed that velocity is found to decrease with the increase in scadmith number Sc.

**Fig 1c:** Velocity profiles for various values of reaction rate parameter γ

Figure 1c shows that the effect of reaction rate parameter on velocity profiles. Considering β=1.0, Sc=0.5 and reaction rate parameter γ at 0.0, 1.0 and 2.0, it is observed that velocity is found to decrease with the increase in reaction rate parameter.
**Fig 2a:** Variation of concentration for several values of casson parameter

Figure 2a shows that the effect of casson parameter on concentration profiles. Considering $\gamma=0.0, \text{Sc}=1.0$ and Casson parameter $\beta$ at 0.5, 1.0 and 2.0, it is observed that concentration is found to be increasing with the increase in Casson parameter $\beta$.

**Fig 2b:** Variation of concentration with $\eta$ for several values of Schmidt number in presence of destructive chemical reaction

Figure 2b and 2c shows that the effect of Schmidt number on concentration profiles. Considering $\gamma=0.1, \beta=2.0$ and scadmith number Sc at 0.5, 1.0 and 1.5, it is observed that concentration is found to be decreasing with the increase in Schmidt number Sc in presence of destructive chemical reaction and for $\gamma=0.0, \beta=2.0$ and scadmith number Sc at 0.5, 1.0 and 1.5, it is observed that concentration is found to be
decreasing with the increase in Schmidt number $Sc$ in absence of chemical reaction.

**Fig 2c:** Variation of concentration with $\eta$ for several values of Schmidt number in absence of chemical reaction

![Graph](image)

**Fig 2d:** Variation of concentration with $\eta$ for several values of reaction parameter $\gamma$

![Graph](image)

Figure 2d shows that the effect of reaction rate parameter on concentration profiles. Considering $\beta=2.0, Sc=0.5$ and reaction rate parameter $\gamma$ at 0.0, 0.3 and 0.6, it is observed that Concentration is found to be decreasing with the increase in reaction rate parameter $\gamma$. 
CONCLUSIONS:
In this present investigation, it is observed that

1. Velocity is found to decrease with the increasing Casson parameter \( \beta \), Scadsmith number \( Sc \) and reaction rate parameter \( \gamma \).

2. Concentration is found to be increasing with the increase in Casson parameter \( \beta \).

3. Concentration is found to be decreasing with the increase in Schmidt number \( Sc \) in presence of destructive chemical reaction and in absence of chemical reaction.

4. Concentration is found to be decreasing with the increase in reaction rate parameter \( \gamma \).

REFERENCES


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