Effect of chemical reaction and heat generation on 3D double diffusive convection over a stretching plate: Numerical and analytical study

S Eswaramoorthi$^1$ S Sivasankaran$^{2, a}$ and Ali Saleh Alshomrani$^2$

$^1$Department of Mathematics, Dr. N. G. P. Arts and Science College, Coimbatore 641 048, Tamil Nadu, India
$^2$Department of Mathematics, King Abdulaziz University, Saudi Arabia
E-mail: $^a$sd.siva@yahoo.com

Abstract. The heat absorption/generation and chemical reaction effects of unsteady flow of a viscous fluid over a stretching plate is analyzed. The governing PDF models are converted into an ODE model with the help of similarity variable and they are solved analytically using the homotopy analysis method (HAM) and numerically by Runge-Kutta fourth order method. The skin-friction coefficient, local Nusselt and local Sherwood numbers are tabulated for various values of the parameters. It is observed that the heat transfer gradient rises on strengthening the heat absorption/generation parameter and it suppresses on escalating the stretching ratio parameter. The mass transfer gradient increases on rising the chemical reaction parameter and it diminishes on rising the unsteady parameter.

Keywords: heat/mass transfer, homotopy analysis method, chemical reaction, heat absorption/generation.

1. Introduction
The heat-mass transfer over a stretching plate is essential in many practical applications in science and engineering. Some applications are hot rolling, glass wire production, glass blowing and fibers spinning, etc. Wang[1] analyzed the 3D flow over a flat surface. Unsteady magnetohydrodynamic flow in a porous stretching surface was examined by Hayat et al.[2]. They found that the temperature drops on rising the Prandtl number. The heat-mass transfer effects of a viscoelastic fluid was analytically studied by Eswaramoorthi et al. [3]. They found that the heat transfer gradient depresses as enlarging the radiation parameter. Various authors discussed in this problem in different aspects, see ([4]-[7]).

The effect chemical reaction is important in many chemical engineering processes, like, food processing, solar collector, formation and dispersion of fog, etc. Hayat et al.[8] examined the second grade fluid flow with chemical reaction and found that, upgrading the fluid concentration due to raising the chemical reaction parameter. The chemically reacting viscoelastic fluid flow was investigated by Cortell et al.[9]. Few significant analysis in this direction is highlighted in ([10] -[17]).

The aim of this paper is to study the mass and heat transfer of unsteady 3D fluid flow with chemical reaction and heat absorption/generation over a time dependent stretching surface.
Our present study is to extend the work of Aboeldahab et al. [11] to include heat generation and absorption parameter.

2. Mathematical Formulation

Consider the 3D flow of a viscous fluid with mass and heat transfer over a stretching plate. Let \( x_1 \& x_2 \) axes be taken in the plate and the \( x_3 \) axis is chosen normal to it. The plate is inclined at an angle \( \alpha \) with the horizontal line. The governing boundary layer equations can be defined as, see, Aboeldahab et al. [11],

\[
\begin{align*}
 u_{x_1} + v_{x_2} + w_{x_3} &= 0 \\
 u_t + u u_{x_1} + v u_{x_2} + w u_{x_3} &= \nu u_{x_1 x_1} + [\beta_1(T - T_\infty + \beta_2(C - C_\infty))] g \cos \alpha \\
 v_t + u v_{x_1} + v v_{x_2} + w v_{x_3} &= \nu v_{x_2 x_2} + [\beta_1(T - T_\infty + \beta_2(C - C_\infty))] g \sin \alpha \\
 T_t + u T_{x_1} + v T_{x_2} + w T_{x_3} &= \frac{k}{\rho c_p} T_{x_1 x_1} + \frac{S}{\rho c_p} (T - T_\infty) \\
 C_t + u C_{x_1} + v C_{x_2} + w C_{x_3} &= DC_{x_1 x_1} + \Gamma (C - C_\infty)^n
\end{align*}
\]

where \( u, v, w, \nu, \beta_1 & \beta_2, g, T, T_w, T_\infty, C, C_w, C_\infty, k, \rho, c_p, S, D, \Gamma \) & \( n \) are the velocity components in \( x_1, x_2 \& x_3 \) directions, kinematical viscosity, thermal and concentration expansion coefficients, acceleration due to gravity, temperature, temperature at the plate, ambient fluid temperature, concentration, concentration at the plate, ambient fluid concentration, thermal conductivity, density, specific heat, heat generation/absorption coefficient, mass diffusivity, chemical reaction time rate & order, respectively.

The initial and boundary conditions are given by:

\[
\begin{align*}
 u(x_1, x_2, x_3, 0) &= u_i, \quad v(x_1, x_2, x_3, 0) = v_i, \quad w(x_1, x_2, x_3, 0) = w_i, \\
 T(x_1, x_2, x_3, 0) &= T_i, \quad \text{and} \quad C(x_1, x_2, x_3, 0) = C_i.
\end{align*}
\]

For \( t > 0 \)

\[
\begin{align*}
 u(x_1, x_2, 0, t) &= ax_1, \quad v(x_1, x_2, 0, t) = bx_2, \quad w(x_1, x_2, 0, t) = 0, \\
 T(x_1, x_2, 0, t) &= T_w, \quad C(x_1, x_2, 0, t) = C_w. \\
 u(x_1, x_2, \infty, t) &= v(x_1, x_2, \infty, t) = w(x_1, x_2, \infty, t) = 0 \\
 T(x_1, x_2, \infty, t) &= T_\infty, \quad C(x_1, x_2, \infty, t) = C_\infty.
\end{align*}
\]

where \( u_i, v_i, w_i, T_i, C_i \) are functions of \( x, y, z \) and \( a_0, b_0, T_w, C_w, T_\infty, C_\infty \) are constants,

\[
\begin{align*}
 a &= a_0(1 - \lambda a_0 t)^{-1}, \quad b = b_0(1 - \lambda a_0 t)^{-1}, \quad T_w = T_w(1 - \lambda a_0 t)^{-2}, \\
 C_w &= C_w(1 - \lambda a_0 t)^{-2}, \quad T_\infty = T_\infty(1 - \lambda a_0 t)^{-2} \quad \text{and} \quad C_\infty = C_\infty(1 - \lambda a_0 t)^{-2}.
\end{align*}
\]

It is interesting to note that the mathematical model (1) - (7) is studied without heat and mass transfer by Wang [1] and it is investigated without mass transfer by Lakshmisha et al. [4]. Aboeldahab et al. [11] extended this work by including mass transfer with chemical reaction without heat generation or absorption.
Substituting equation (8) into equations (1) - (7), the following similarity equations are obtained.

\[
\begin{align*}
\eta(z, t) &= \sqrt{a_0/vz(1 - \lambda t)}^{-\frac{1}{2}}, \quad t = a_0 t, \quad \lambda t < 1, \\
u[x, \eta(z, t)] &= [A \cos \alpha f(\eta) + a_0 x g'(\eta)](1 - \lambda t)^{-1}, \\
v[y, \eta(z, t)] &= [A \sin \alpha r(\eta) + a_0 y s'(\eta)](1 - \lambda t)^{-1}, \\
w[\eta(z, t)] &= \sqrt{a_0/v[g(\eta) + s(\eta)](1 - \lambda t)^{-\frac{3}{2}},} \\
A &= \frac{g[\beta_T(T_w - T_{\infty}) + \beta_C(C_{w0} - C_{\infty})]}{a_0}, \\
\theta[\eta(z, t)] &= \frac{T - T_{\infty}}{T_{w0} - T_{\infty}} (1 - \lambda t)^{2} \quad \text{and} \quad \phi[\eta(z, t)] = \frac{C - C_{\infty}}{C_{w0} - C_{\infty}} (1 - \lambda t)^{2}.
\end{align*}
\]  

Substituting equation (8) into equations (1) - (7), the following similarity equations are obtained.

\[
\begin{align*}
f'' + (g + s)f' - g' f + \frac{\theta + N \phi}{1 + N} - \lambda(f + \eta \frac{\eta f'}{2}) &= 0, \\
g'' + (g + s)g'' - g' g'' - \lambda(g' + \eta \frac{\eta g''}{2}) &= 0, \\
r'' + (g + s)r' - s'r + \frac{\theta + N \phi}{1 + N} - \lambda(r + \eta \frac{\eta r'}{2}) &= 0, \\
s'' + (g + s)s'' - s' s'' - \lambda(s' + \eta \frac{\eta s''}{2}) &= 0, \\
\theta'' + Pr \left[(g + s)\theta' - \lambda(2\theta + \eta \frac{\eta \theta'}{2}) + Q\theta\right] &= 0, \\
\phi'' + Sc \left[(g + s)\phi' - \lambda(2\phi + \eta \frac{\eta \phi'}{2}) + \gamma_0 \phi\right] &= 0
\end{align*}
\]  

| c   | \(-g''(0)\) | \(-s''(0)\) | \(-\theta'(0)\) |
|-----|--------------|--------------|------------------|
|     | HAM         | Numerical    | Ref. [11] HAM    | R-K | Ref. [11] HAM | R-K | Ref. [11] |
| 0.0 | 1.0000000   | 1.0000000   | 1.0000000 0.0000000 | 0.0000000 | 0.45444 | 0.45444 | 0.45444 |
| 0.25| 1.04885     | 1.04850     | 1.04885 0.19464 | 0.19450 | 0.19464 | 0.52090 | 0.52100 | 0.52110 |
| 0.50| 1.09301     | 1.09301     | 1.09310 0.46520 | 0.46530 | 0.46520 | 0.57570 | 0.57580 | 0.57580 |
| 0.75| 1.13450     | 1.13450     | 1.13450 0.79464 | 0.79450 | 0.79464 | 0.62370 | 0.62370 | 0.62380 |
| 1.00| 1.17371     | 1.17371     | 1.17371 1.17371 | 1.17371 | 1.17371 | 0.66730 | 0.66720 | 0.66730 |

The boundary conditions are given by:

\[
\begin{align*}
f(0) &= r(0) = g(0) = s(0) = 0, \quad g'(0) = \theta(0) = \phi(0) = 1, \\
s'(0) &= \frac{b_0}{a_0} = c, \quad f(\infty) = r(\infty) = g(\infty) = s(\infty) = 0, \\
g'(\infty) &= s'(\infty) = \theta(\infty) = \phi(\infty) = 0
\end{align*}
\]  

The dimensionless number appeared in the above equations are defined as follows.

\[
N = \frac{Gr_C}{Gr_T} = \frac{\beta_C(C_{w0} - C_{\infty})}{\beta_T(T_w - T_{\infty})}, \quad Pr = \frac{\mu c_p}{k}, \quad Gr_C = \frac{g^3 \beta C(C_{w0} - C_{\infty})}{\nu^2}, \\
Gr_T = \frac{g^3 \beta T(T_w - T_{\infty})}{\nu^2}, \quad Sc = \frac{\nu}{D}, \quad \gamma_0 = \frac{\Gamma_0(C_{w0} - C_{\infty})^{\frac{n-1}{2}}}{a_0} \quad \text{and} \quad \nu = \frac{\mu}{\rho}.
\]
IOP Conf. Series: Journal of Physics: Conf. Series 1139 (2018) 012001
doi:10.1088/1742-6596/1139/1/012001

Table 2. Nusselt and Sherwood numbers for different parameters with $N = 1.0$, $Pr = 0.7$, and $Sc = 0.3$

| $\lambda$ | $\gamma_0$ | $c$ | $Q$ | $-\theta'(0)$ | $-\phi'(0)$ |
|-----------|-------------|-----|-----|---------------|--------------|
| -0.5      | -0.2        | 0.5 | 0.3 | 3.860323      | 3.860325     |
| -0.2      | -0.5        | 0.3 |     | 0.328177      | -0.260736    |
| 0.0       |             |     |     | -0.284261     | -0.412970    |
| 0.2       |             |     |     | -0.581103     | -0.528998    |
| 0.5       |             |     |     | -0.851794     | -0.665831    |
| -0.2      | -0.2        | 0.5 | 0.3 | 0.328177      | -0.404029    |
| 0.1       |             |     |     | 0.965307      | -0.212764    |
| 0.5       |             |     |     | 0.328177      | -0.260736    |
| 1.0       |             |     |     | -0.056688     | -0.308987    |
| -0.2      | -0.2        | 0.5 | -0.5| -0.690923     | -0.260736    |
| 0.0       |             |     |     | -0.317897     | -0.260736    |
| 0.3       |             |     |     | 0.328177      | -0.260736    |
| 0.5       |             |     |     | 1.848729      | -0.260736    |

The local Nusselt and Sherwood numbers are important quantities in engineering applications. So, the local Nusselt and Sherwood numbers are defined by

$$Nu/\sqrt{Re_x(1-\lambda t)}^\frac{3}{2} = -\theta'(0),$$
$$Sh/\sqrt{Re_x(1-\lambda t)}^\frac{3}{2} = -\phi'(0)$$

3. Analytical Solutions

Equations (9) to (14) with (15) are solved analytically using HAM. These HAM solutions depend upon $h_f$, $h_g$, $h_r$, $h_s$, $h_\theta$ & $h_\phi$ parameters, see([15]-[17]) and these parameters depend on $f'(0), g''(0), r'(0), s'(0), \theta'(0)$ and $\phi'(0)$. Figures 1(a) and 1(b) show the range values of $h_f$ & $h_r$ and $h_g$ & $h_s$ are $-1.2 \leq h_f, h_r \leq -0.7$ and $-1.5 \leq h_g, h_s \leq -0.4$. Figure 1(c) represents the value of $h_\theta$ & $h_\phi$ are $-1.6 \leq h_\theta \leq -0.7$ and $-1.6 \leq h_\phi \leq -0.6$. We fix $h_f = h_g = h_r = h_s = h_\theta = h_\phi = -1.0$ for better solution.

4. Numerical Solutions

Solving the nonlinear ordinary differential equations (9) to (14) is more critical. The resulting system of equations with the boundary conditions (15) are numerically solved using Runge-Kutta fourth order method & Shooting technique with initial guessing $f'(0), g'(0), r'(0), s''(0), \theta'(0)$ and $\phi'(0)$. This process is repeated until we get the required degree of accuracy of $10^{-6}$. The analytical and numerical results are compared with the results existing in the literature and they are shown in the Table 1. This provides the assurance of our analytical and numerical results to be used in the subsequent problem.
Figure 1. h curves of $f'(0)$ & $r'(0)$ (a), $g''(0)$ & $s''(0)$ (b) and $\theta'(0)$ & $\phi'(0)$ (c) with $N = 1.0, \lambda = -0.1, Q = -0.3, \gamma_0 = -0.2$ and $c = 0.5$

Figure 2. The variations of $f$ (a) and $r$ (b) for different values of $N$ with $\lambda = -0.1, Q = -0.3, \gamma_0 = -0.2$ and $c = 0.5$
Figure 3. The variations of $f$ (a) and $r$ (b) for different values of $\lambda$ with $N = 1.0, Q = -0.3, \gamma_0 = -0.2$ and $c = 0.5$

Figure 4. The variations of $f$ (a) and $r$ (b) for different values of $Q$ with $N = 1.0, \lambda = -0.1, \gamma_0 = -0.2$ and $c = 0.5$

Figure 5. The variations of $f$ (a) and $r$ (b) for different values of $(\gamma_0)$ with $N = 1.0, \lambda = -0.1$ and $c = 0.5$
Figure 6. The variations of $\theta$ (a) and $\phi$ (b) for different values of $\lambda$ with $N = 1.0, Q = -0.3, \gamma_0 = -0.2$ and $c = 0.5$

Figure 7. The variations of $\theta$ for different values of $Q$ with $N = 1.0, \lambda = -0.1, \gamma_0 = -0.2$ and $c = 0.5$

Figure 8. The variations of $\phi$ for different values of $(\gamma_0)$ with $N = 1.0, \lambda = -0.1, Q = -0.3$ and $c = 0.5$
5. Results and Discussion
In this section, we present the graphical results of \( f, g', r, s', \theta \) and \( \phi \) for different combinations of the pertinent parameters with constant values of \( Pr(=0.71) \) and \( Sc(=0.3) \). The calculated values of local Nusselt and Sherwood numbers for unsteady parameter \( \lambda \), chemical reaction parameter \( \gamma_0 \), stretching ratio \( c \) and heat generation or absorption parameter \( Q \) are presented in Table 2. It is observed from the table that the increasing values of \( \lambda \) and \( c \) is to reduce the local Nusselt and Sherwood numbers. There is no change in heat transfer when changing the values of \( \gamma_0 \). The rate of mass transfer is independent of \( Q \). Further, the value \( Nu \) enhances with rising the values of \( Q \) and \( Sh \) value boosted up with enhancing the values of \( \gamma_0 \). Figures 2(a) & 2(b) show the effects of \( N \) on velocity profiles and seen that the velocities and their associated boundary layer thicknesses reduce with enhancing the buoyancy ratio parameter. The various values of \( \lambda \) on velocity profiles are displayed in figures 3(a) & 3(b). It is evident that the velocity boundary layer thicknesses reduce monotonically when the unsteady parameter increases. This shows the velocity gradient improving when increasing the unsteady parameter.

Figures 4(a) & 4(b) display the effects of \( Q \) on velocity profiles. It is found that the positive values of \( Q \) leads to strengthen the thickness velocity boundary layer and the negative values of \( Q \) causes the weaken the thickness velocity boundary layer. The variations of chemical reaction parameter \( \gamma_0 \) on velocity profiles are shown in figures 5(a) & 5(b). It is seen from these figures that chemical reaction parameter enlarge the velocities and their associated boundary layer thicknesses. Figures 6(a) & 6(b) illustrate the variations of \( \lambda \) on \( \theta \) and \( \phi \). It is found that the fluid temperature and fluid concentration reduces when unsteady parameter increases. The effect of \( Q \) on \( \theta \) is shown in figure 7. It is expected that the heat generation \( (Q > 0) \) got thickening of the thermal boundary layer because of the fluid is warmer. However, the heat absorption \( (Q < 0) \) got thinning the thermal boundary layer that the fluid gets cooler. It is evident from figure 8 that the destructive chemical reaction \( (\gamma_0 > 0) \) makes the thicken the concentration boundary layer as well as increase the species concentration, but the generative chemical reaction \( (\gamma_0 < 0) \) reduces the species concentration and it leave the concentration boundary layer to be thinner.

6. Conclusions
In this paper, we investigate the 3D double diffusive convective flow with heat-mass on a stretching plate with heat generation and chemical reaction. An analytical solution based on HAM and numerical solution by RK method are obtained. The heat-mass transfer rates are also calculated. The main observations are listed below. The fluid velocity drops when rising the unsteadiness parameter. The fluid temperature reduces when increasing the unsteady parameter. The fluid concentration enhances when rising the values of \( \gamma_0 \). The value \( Nu \) enhances with increasing the values of \( Q \) and it suppresses on enhancing the values of \( \lambda \) and \( c \). The value \( Sh \) improves on enhancing \( \gamma_0 \) values and it depress on increasing values of \( \lambda \) and \( c \).

References
[1] Wang C Y 1984 The three-dimensional flow due to a stretching flat surface Phys. Fluids 27 pp 1915-1917
[2] Hayat T, Qasim M and Abbas Z 2010 Homotopy solution for the unsteady three-dimensional MHD flow and mass transfer in a porous space. Commun. Nonlinear Sci. Numer. Simulat. 15 pp 2375-2387
[3] Eswaramoorthi S, Bhuvaneswari M, Sivasankaran S and Rajan S 2016 Soret and Dufour effects on viscoelastic boundary layer flow, heat and mass transfer in a stretching surface with convective boundary condition in the presence of radiation and chemical reaction Scientia Iranica -Trans. B:Mech. Eng. 23(6), pp 2575-86
[4] Lakshmisha KN, Venkateshwaran S and Nath G 1988 Three dimensional unsteady flow with heat and mass transfer over a continuous stretching surface. J. Heat Transf. 115, 590-595
[5] Sivasankaran S, Niranjana H and Bhuvaneswari M 2017 Chemical reaction, radiation and slip effects on MHD mixed convection stagnation point-flow in a porous medium with convective boundary condition Int. J. Numer. Meth. Heat Fluid Flow 27 pp 454-470
[6] Bhuvaneswari M, Sivasankaran S and Kim YJ 2012 Lie group analysis of radiation natural convection flow over an inclined surface in a porous medium with internal heat generation J. Porous Media 15 pp 1155-1164

[7] Motsa SS, Shateyi S and Makukula Z 2011 Homotopy analysis of free convection boundary layer flow with heat and mass transfer Chem. Eng. Comm. 198 pp 783-795

[8] Hayat T, Abbas Z and Sajid M 2008 Heat and mass transfer analysis on the flow of a second grade fluid in the presence of chemical reaction Phys. Lett. A 372 pp 2400-2408

[9] Cortell R 2007 Toward an understanding of the motion and mass transfer with chemically reactive species for two classes of viscoelastic fluid over a porous stretching sheet Chem. Eng. Process. 46 pp 982-989

[10] Niranjan H, Sivasankaran S, and Bhuvaneswari M 2017 Chemical reaction, Soret and Dufour effects on MHD mixed convection stagnation point flow with radiation and slip condition Scientia Iranica Transaction of Mechanical Engineering B 24 pp 698-706

[11] Aboeldahab EM and Azzam GE-DA 2006 Unsteady three-dimensional combined heat and mass free convective flow over a stretching surface with time-dependent chemical reaction Acta Mech. 184 pp 121-136

[12] Karthikeyan S, Bhuvaneswari M, Sivasankaran S and Rajan S 2016 Soret and Dufour effects on MHD mixed convection heat and mass transfer of a stagnation point flow towards a vertical plate in a porous medium with chemical reaction, radiation and heat generation J. Appl.Fluid Mech. 9 pp 1447-155

[13] Kasmani RM, Sivasankaran S, Bhuvaneswari M and Siri Z 2016 Effect of chemical reaction on convective heat transfer of boundary layer flow in nanofluid over a wedge with heat generation/absorption and suction J. Appl. Fluid Mech. 9 pp 379-388

[14] Bhuvaneswari M, Sivasankaran S and Ferdows M Lie group analysis of natural convection heat and mass transfer in an inclined surface with chemical reaction Non-lin. Anal. Hybrid Sys. 3 pp 536-542

[15] Eswaramoorthi S, Bhuvaneswari M, Sivasankaran S and Makinde OD 2018 Heterogeneous and homogeneouse reaction analysis on MHD Oldroyd-B fluid with Cattaneo-Christov heat flux model and convective heating Def. Diff. Forum 387 pp 194-206

[16] Niranjan H, Sivasankaran S and Bhuvaneswari M 2016 Analytical and numerical study on magnetoconvection stagnation-point flow in a porous medium with chemical reaction, radiation and slip effects Math. Prob. Eng. Article ID 4017076 pp 1-12

[17] Eswaramoorthi S, Bhuvaneswari M, Sivasankaran S and Rajan S 2015 Effect of radiation on MHD convective flow and heat transfer of a viscoelastic fluid over a stretching surface Procedia Eng. 127 pp 916-923