



HEAT AND MASS TRANSFER DUE TO DOUBLE DIFFUSIVE MIXED CONVECTION IN A PARALLEL PLATE REACTOR IN PRESENCE OF CHEMICAL REACTION AND HEAT GENERATION

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ABSTRACT

The present paper aims to analyze numerically the heat and mass transfer for laminar double-diffusive mixed convection flow in a parallel plate reactor with heat generation and chemical reaction. The reactant fluid enters from the left inlet and exits from the right outlet. All solid walls of the reactor are assumed to be thermodynamically isolated. After entering the reactor, the fluid passes four heated cylinder. Two-dimensional continuity, momentum, energy and concentration equations govern the developed mathematical model. Galerkin finite element method with triangular grid discretization system is used to solve the governing non-dimensional equations. The aim of the investigation is to illustrate the effects of the energy expelled during the reaction, on velocity, the thermal field and concentration of the heat sensitive chemical. Numerical simulations are conducted for different combinations of chemical reaction parameter and heat generation parameter. Results are presented in terms of streamlines, temperature and concentration distributions. The results reveal that the heat and mass transfer rate strongly depend on the mentioned parameter.

Keywords: Double diffusive mixed convection, Parallel plate reactor, Heat generation, Chemical reaction, Finite element, Heat transfer, Mass transfer.

Contribution/ Originality

This study is one of very few studies which have investigated the heat and mass transfer in a chemical reactor using finite element method. The paper's primary contribution is finding the effect of chemical reaction and heat generation on the flow temperature and concentration in a parallel plate reactor.

1. INTRODUCTION

There are many transport processes governed by the joint action of both thermal and mass diffusion in the presence of chemical reaction effects including many engineering applications such as nuclear reactor safety, combustion systems, solar collectors, metallurgy, and chemical engineering. Representative applications of interest include: solidification of binary alloy and crystal growth, dispersion of dissolved materials or particulate water in flows, drying and dehydration operations in chemical and food processing plants, and combustion of atomized liquid fuels. Furthermore, the presence of a foreign mass in air or water causes some kind of chemical reaction. During a chemical reaction between two species heat is also generated. Therefore combined heat and mass transfer problems with chemical reaction and heat generation received a considerable amount of attention in recent years.

Double diffusion on free/mixed convection flow is widely used by the researchers. [Salma, et al. \[1\]](#) analyzed numerically the effect of double-diffusive natural convection of water–Al₂O₃ nanofluid. They analyzed Soret and Dufour coefficients in a partially heated enclosure. A numerical study was done by [Brown and Lai \[2\]](#), where they investigated combined heat and mass transfer of a horizontal channel with an open cavity heated from below. Double diffusive mixed convection in an open channel was investigated by [Azad, et al. \[3\]](#). They used a circular heater on the bottom wall and found that decreased the average Nusselt number at the heat source and overall mass transfer rate in terms of average Sherwood number increased when the Lewis number rose. The steady-state laminar mixed convection of a binary gas mixture in a parallel-plate channel was investigated by [Kiari Goni, et al. \[4\]](#). This paper presented an exact analytical solution for the fully developed flow problem in parallel with the numerical effort which proven to be of great value for validation purposes. [Oulaid, et al. \[5\]](#) adopted the same mathematical model and proposed criteria for flow reversal in terms of the Reynolds number and the thermal and solutal Grashof numbers.

The effect of the chemical reaction and injection for the flow characteristics was analyzed by [Muthucumaraswamy and Ganesan \[6\]](#). They considered an unsteady upward motion of an isothermal plate. The result shows that chemical reaction parameter increased when the fluid velocity decreased. They also analyzed the distributions of local and averaged values of skin friction and Nusselt and Sherwood numbers. [Das, et al. \[7\]](#) studied the unsteady flow past an infinite vertical plate with a constant heat and mass transfer. They considered the effect of the first order homogeneous chemical reaction on the process. The result indicated that the velocity decreases but the skin-friction being positive at large values of the chemical reaction parameter because of the presence of first order chemical reaction. [Chamka \[8\]](#) numerically investigated the MHD flow of a uniformly stretched vertical permeable surface in the presence of heat generation/absorption and a chemical reaction. He assumed that the plate was embedded in a uniform porous medium and moved with a constant velocity in the flow direction in the presence of a transverse magnetic field.

An Analytical solution on heat and mass transfer with laminar flow of a Newtonian, viscous fluid had been done by Ibrahim, et al. [9]. He analyzed the effect of chemical reaction and radiation absorption on the unsteady MHD free convection flow past a semi-infinite vertical permeable moving plate with heat source and suction. They analyzed numerically and the graphical results illustrated the flow and heat and mass transfer characteristics in details and their dependence on some of the physical parameters. They found that the velocity profiles increased because of decreasing chemical reaction parameter, the Schmidt number, heat absorption coefficient, magnetic field. Also they found that the concentration profile increased due to decrease in the chemical reaction parameter c and the Schmidt number Sc . Heat and mass transfer of an unsteady MHD convective flow past a semi-infinite vertical permeable moving plate was studied by Kesavaiah, et al. [10]. They observed the effect of the chemical reaction and radiation absorption on the plate embedded in a porous medium with heat source and suction. Abiodun, et al. [11] studied the diffusion-thermo and chemical reaction effects on unsteady MHD flow between two inclined parallel plates with heat source and radiation absorption. They found that, the velocity profiles decreased with increase in chemical reaction and magnetic field parameter while increased in Dufour parameter, buoyancy ratio and permeability parameters boost the velocity profiles. Patil, et al. [12] investigated the steady, laminar mixed convection flow over a continuously moving semi-infinite vertical plate due to the combined effects of thermal and mass diffusion in the presence of internal heat generation or absorption and an n th order homogeneous chemical reaction between the fluid and the diffusing species. Swapna, et al. [13] studies the steady, two-dimensional, heat and mass transfer flow of a chemically reacting mixed convection of magneto-micropolar fluid over a wedge with a convective surface boundary condition. The study finds applications in chemical reaction engineering processes, magnetic materials processing, solar collector energy systems, etc. Heat and mass transport in tubular packed reactors at reacting and non-reacting conditions were analyzed by Koning [14] where the most common models of wall-cooled tubular packed bed reactors were presented. The two dimensional axial plug flow model was used for a water gas shift reactor to compare heat conduction or mass diffusion with convective effect. The result showed the values of the effective heat transport parameters obtained from experiments at reacting conditions may be different from those obtained from experiments without reaction. Kugai [15] studied the heat and mass transfer in a fixed-bed tubular reactor. The two dimensional axial plug flow model was used for a water gas shift reactor to compare heat conduction or mass diffusion with convective effect in his study. The objective of the present work is to investigate the effect of chemical reaction and heat generation/absorption on the double-diffusive mixed convection in a parallel plate reactor. Streamlines, isotherms and iso-concentrations, heat and mass transfer rate, average velocity, temperature and concentration are analyzed for the comprehensive study.

2. ANALYSIS

2.1. Physical Model

The domain under analysis is, as sketched in Figure 1(a)-(b), a two-dimensional cross section of a reactor channel of length L and height H with four heated tubes each of radius r , suffering the influence of a gravitational field. The centers of the heaters are located at $(L/5, H/2)$, $(2L/5, H/2)$, $(3L/5, H/2)$ and $(4L/5, H/2)$. The heaters are maintained at a constant and uniform temperature T_h . The flow is entering from the left with velocity U_i , temperature T_i and concentration C_i , then passes the tubes and then exhausted from the outlet opening at the right.

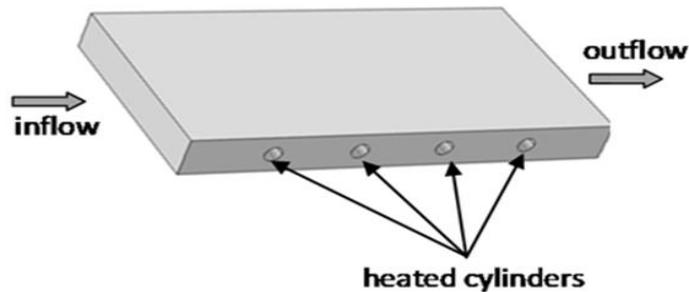


Fig-1(a). 3-D geometry of the considered reactor

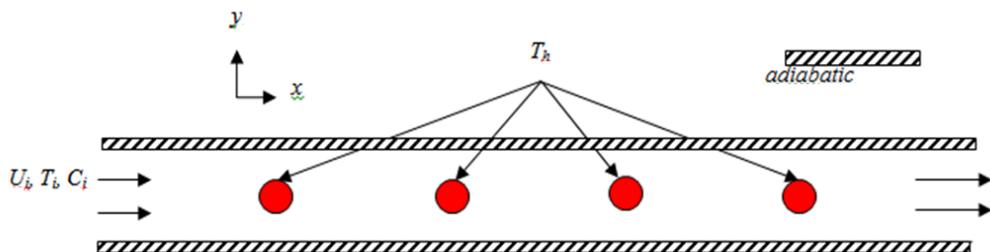


Fig-1(b). Schematic diagram of the problem

2.2. Mathematical Model

The governing mass, momentum, energy and species conservation equations have been presented by Deng, et al. [16] for double-diffusive mixed convective flows driven by the combined effect of the internal buoyancy induced from temperature and concentration differences and the external mechanical driven forced flow from the inlet port. With use of the Boussinesq approximation, the dimensionless governing equations under steady-state condition are given by:

$$\text{Continuity equation: } \frac{\partial U}{\partial X} + \frac{\partial V}{\partial Y} = 0$$

$$\text{X-momentum equation: } U \frac{\partial U}{\partial X} + V \frac{\partial U}{\partial Y} = -\frac{\partial P}{\partial X} + \frac{1}{Re} \left(\frac{\partial^2 U}{\partial X^2} + \frac{\partial^2 U}{\partial Y^2} \right)$$

$$\text{Y-momentum equation: } U \frac{\partial V}{\partial X} + V \frac{\partial V}{\partial Y} = -\frac{\partial P}{\partial Y} + \frac{1}{Re} \left(\frac{\partial^2 V}{\partial X^2} + \frac{\partial^2 V}{\partial Y^2} \right) + Ri(\theta + NC)$$

$$\text{Energy equation: } U \frac{\partial \theta}{\partial X} + V \frac{\partial \theta}{\partial Y} = \frac{1}{RePr} \left(\frac{\partial^2 \theta}{\partial X^2} + \frac{\partial^2 \theta}{\partial Y^2} \right) - \gamma \theta$$

$$\text{Diffusion equation: } U \frac{\partial C}{\partial X} + V \frac{\partial C}{\partial Y} = \frac{1}{RePrLe} \left(\frac{\partial^2 C}{\partial X^2} + \frac{\partial^2 C}{\partial Y^2} \right) - KC$$

The above equations are non-dimensionalized by using the following dimensionless variables

$$X = \frac{x}{L}, Y = \frac{y}{L}, U = \frac{u}{U_i}, V = \frac{v}{U_i}, P = \frac{p}{\rho U_i^2}, \theta = \frac{T - T_i}{T_h - T_i}, C = \frac{c - C_i}{\Delta c}$$

and the dimensionless parameters are Reynolds number (Re), Grashof number (Gr), Richardson number (Ri), Prandtl number (Pr), Lewis number (Le), the buoyancy ratio (N), heat source parameter (γ) and Chemical reaction parameter (K) and they are defined as follows:

$$Re = \frac{U_i L}{\nu}, Gr = \frac{g \beta_T (T_h - T_i) L^3}{\nu^2}, Ri = \frac{Gr}{Re^2}, Pr = \frac{\nu}{\alpha}, Le = \frac{\alpha}{D}, N = \frac{\beta_c \Delta c}{\beta_T (T_h - T_i)}$$

$$, \gamma = \frac{QL^2}{\alpha}, K = \frac{kL^2}{D}$$

where ν , α , D , k and Q are kinematic viscosity, thermal diffusivity, solutal diffusivity, reaction coefficient and strength of heat generating source respectively. The buoyancy ratio measures the relative importance of solute and thermal diffusion in creating the density difference to drive the flow. It is clear that N is zero for pure thermally driven flows and infinity for pure solute driven flows.

The boundary conditions are

at the inlet: $U = 1, V = \theta = C = 0$

at the circular tube walls: $\theta = 1, \frac{\partial C}{\partial n} = 0,$

at other surfaces: $\frac{\partial \theta}{\partial n} = 0, \frac{\partial C}{\partial n} = 0$

at all solid boundaries: $U = V = 0$

Analysis of fluid motion is displayed by means of streamfunction, ψ which is obtained from velocity components U and V . The relationships between streamfunction, ψ and velocity components for two-dimensional flows are

$$U = \frac{\partial \psi}{\partial Y} \text{ and } V = -\frac{\partial \psi}{\partial X}$$

which give a single equation

$$\frac{\partial^2 \psi}{\partial X^2} + \frac{\partial^2 \psi}{\partial Y^2} = \frac{\partial U}{\partial Y} - \frac{\partial V}{\partial X}$$

The positive sign of ψ denotes anticlockwise circulation and the clockwise circulation is represented by the negative sign of ψ . The no-slip condition is valid at all boundaries as there is no cross-flow. Hence $\psi = 0$ is used for boundaries.

The average Nusselt and Sherwood number may be expressed as

$$Nu = -\frac{1}{S} \int_0^S \sqrt{\left(\frac{\partial \theta}{\partial X}\right)^2 + \left(\frac{\partial \theta}{\partial Y}\right)^2} dS \text{ and } Sh = -\frac{1}{S} \int_0^S \sqrt{\left(\frac{\partial C}{\partial X}\right)^2 + \left(\frac{\partial C}{\partial Y}\right)^2} dS$$

The mean velocity, temperature and concentration of the fluid inside the domain are $V_{av} = \int V d\bar{V} / \bar{V}$, $\theta_{av} = \int \theta d\bar{V} / \bar{V}$ and $C_{av} = \int C d\bar{V} / \bar{V}$ respectively. Where S and \bar{V} are the non-dimensional length of the surface and volume of the channel respectively.

3. COMPUTATIONAL METHODOLOGY

The numerical procedure used to solve the governing equations for the present work is based on the Galerkin weighted residual method of finite element formulation. The application of this technique is well documented by [Zienkiewicz and Taylor \[17\]](#). The equation of continuity has been used as a constraint due to mass conservation and this restriction may be used to find the pressure distribution. The finite element method of [Reddy and Gartling \[18\]](#) is used to solve momentum, energy and diffusion equations, where the pressure P is eliminated by a constraint. The continuity equation is automatically fulfilled for large values of this constraint. Then the velocity components (U, V), temperature (θ) and concentration (C) are expanded using a basis set. The

Galerkin finite element technique yields the subsequent nonlinear residual equations. Three points Gaussian quadrature is used to evaluate the integrals in these equations. The non-linear residual equations are solved using Newton–Raphson method to determine the coefficients of the expansions. This approach will result in substantially fast convergence assurance. In addition, the absolute convergence criteria are set to be 10^{-4} for velocities, energy and concentration.

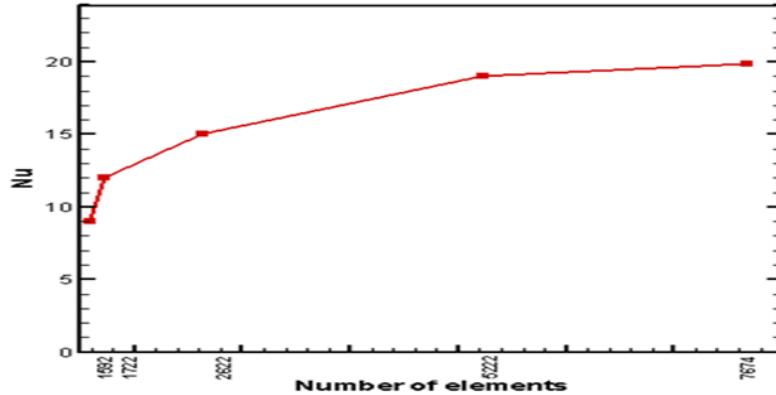


Fig-2. Grid independent test for the geometry

3.1. Grid Independent Test

To guarantee a grid-independent solution, an extensive mesh testing procedure is conducted with $Ri = 1$, $Re = 100$, $Pr = 0.7$, $Le = 1$, $N = 1$, $\gamma = 5$ and $K = 1$ in the considered geometry. In the present work, we examine five different non-uniform grid systems with the following number of elements within the resolution field: 1592, 1722, 2622, 5222 and 7674. The numerical scheme is carried out for highly precise key in the average Nusselt (Nu) number at the first heater for the aforesaid elements to develop an understanding of the grid fineness as shown in Fig. 2. The scale of the average Nusselt numbers for 5222 elements shows a little difference with the results obtained for the higher elements. Hence, the non-uniform grid system of 5222 elements is preferred for the whole computation for saving the computation time.

3.2. Model Validation

The model validation is an important part of a numerical investigation. Hence, the outcome of the present numerical code is benchmarked against the numerical results of [Abiodun, et al. \[11\]](#) which were reported for combined effect of diffusion-thermo and chemical reaction on the unsteady MHD double diffusive flow between two inclined parallel plates with heat and radiation absorption. The comparison is conducted while employing the dimensionless parameters Prandtl number $Pr = 0.71$, chemical reaction parameter $\gamma = 0.6$, Schmidt number $Sc = 0.4$, heat absorption parameter $\lambda = 0.2$, magnetic field parameter $M = 0.2$, radiation absorption parameter $Q = 1$, Dufour parameter $Df = 4$, buoyancy ratio parameter $N = 2$, permeability parameter $K = 2$ and inclination angle $\alpha = \frac{\pi}{4}$. Present results for Average Nusselt number (Nu_0) at $y = 0$ and (Nu_1) at $y = 1$ are shown in Table 1 which is good agreement with those of [Abiodun, et al. \[11\]](#). This validation boosts the confidence in our numerical code to carry on with the above stated objectives of the current investigation.

Table-1. Comparison of Nusselt number for the present numerical technique with that of Abiodun, et al. [11]

	Present result	Abiodun, et al. [11]	Error(%)
Nu_0	0.3298	0.3310	0.36%
Nu_1	1.5507	1.5723	1.37%

4. RESULTS AND DISCUSSION

The present investigation was carried out with controlling parameters: chemical reaction parameter K (0.01, 0.1, 1 and 5) and heat generation parameter γ (0, 1, 5 and 10) while $Re = 100$, $Ri = 1$, $Pr = 0.7$, $Le = 1.5$ and $N = 1$. Now in the following sections, detailed description of mixed convection with heat and mass transfer in a parallel plate reactor is given in terms of streamline, thermal and concentration contours for different K and γ . In addition, the results for average Nusselt and average Sherwood numbers, average velocity, temperature and concentration will be presented.

4.1. Effect on Streamlines

The effects of K and γ on the streamlines are exhibited in Figs 3 (a) – (b). In fact, the analysis is performed at pure mixed convection regime by fixing $Ri = 1$. The values of chemical reaction parameter are 0.01, 0.1, 1 and 5 are chosen to examine the evolution of streamline, isotherm and concentration patterns.

It is observed from Figs. 3(a) - (b), that there is a common trend of the development of streamlines with generating both chemical reaction and heat. The streamlines are almost parallel to the channel wall and condensed in the region between the circular heater and the channel wall. The streamlines become more to less condense along the middle of the channel due to increasing chemical reaction effect while the opposite phenomenon is seen for the increasing heat generation effect. This indicates higher velocity for lower K and higher γ .

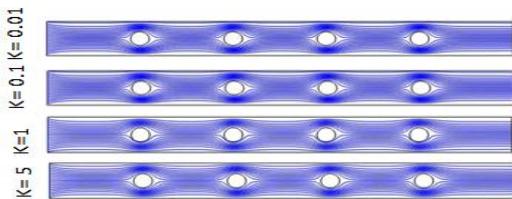


Fig-3(a). Effect of K on streamlines with $\gamma = 5$

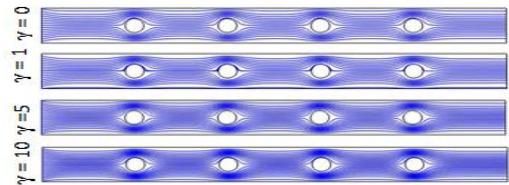


Fig-3(b). Effect of γ on streamlines with $K = 1$

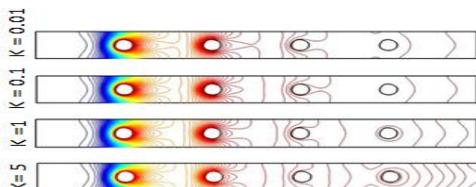


Fig-4(a). Effect of K on isotherms with $\gamma = 5$

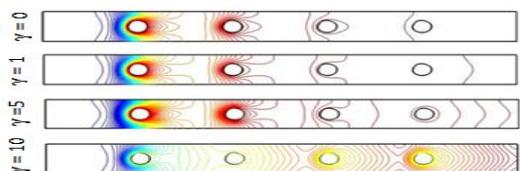


Fig-4(b). Effect of γ on isotherms with $K = 1$

4.2. Effect on Isotherms

From Figs. 4(a)-(b), it is noticed that isothermal lines have considerable change due to the variation of K as well as γ . When there is generating small chemical reaction, lower density of isothermal lines appear at the outlet portion of the channel. But for higher values of K , appearance of these lines is more at the right side. It is seen from the figure that, at the highest value of K , the lower temperature lines remain at the left portion whereas the higher temperature lines at the right exit port. Temperature gradient at the heat source becomes lower for increasing chemical reaction in the fluid. This happens because higher temperature of the fluid produces lower temperature difference between the heat source and the fluid. The similar fact is observable for generating more heat. At $H = 10$, the isothermal lines with higher temperature spreads all over the channel. It is also clear that for both the cases, the higher temperature gradient exists at the first heater from the inlet and sequentially it reduces for the second, third and fourth.

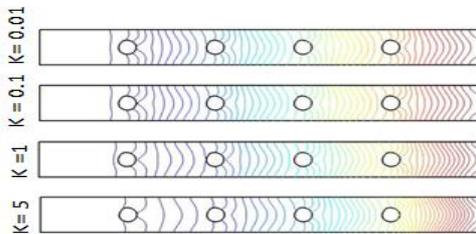


Fig-5(a). Effect of K on iso-concentrations with $\gamma = 5$

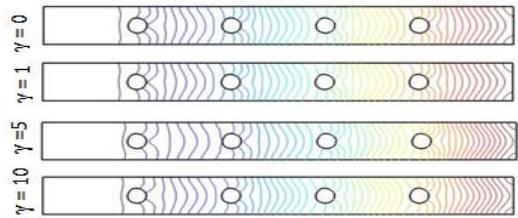


Fig-5(b). Effect of γ on iso-concentrations with $K = 1$

4.3. Effect on Iso-Concentrations

Iso-concentration lines have also substantial change due to heat generation and chemical reaction as shown in Figs. 5(a)-(b). Iso-concentration lines spread all over the channel for all the considered cases. As the values of the parameters increase, these lines depart to the exit port. Higher concentration causes lower concentration gradient which indicates lower mass transportation. Iso-concentration lines become denser for the higher chemical reaction.

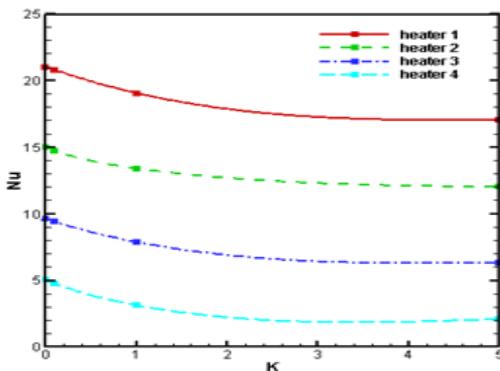


Fig-6(a). Effect of K on heat transfer with $\gamma = 5$

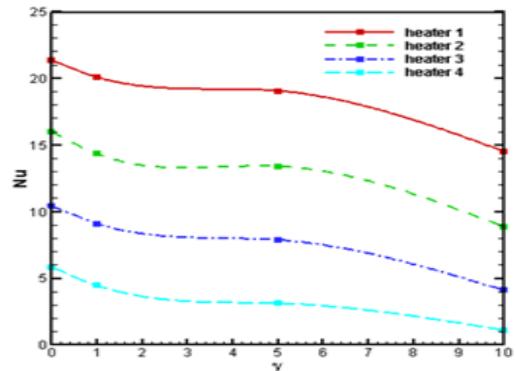


Fig-6(b). Effect of γ on heat transfer with $K = 1$

4.4. Effect on Heat and Mass Transfer

Figs. 6(a)-(b) depicts the average heat transfer Nu at the four consecutive heaters for different K and γ . Highest heat transfer rate is observed for the first heater and sequentially these values reduce for second, third and fourth heater/contaminant. This phenomenon is very logical because the flow intensity becomes lower for the last heater due to the obstacles. Increasing K as well as γ decreases the value of Nu due to lowering the temperature difference. Rate of decrement is more for higher values of γ .

The average mass transfer Sh at the inlet port for various K and γ is shown in Figs. 7(a)-(b). Mass transfer rate decreases for increasing both the chemical reaction and heat generation parameter while the rate of reduction in mass transfer is high for chemical reaction variation.

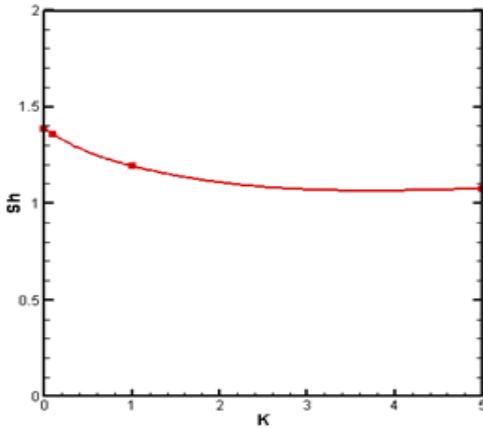


Fig-7(a). Effect of K on mass transfer with $\gamma = 5$

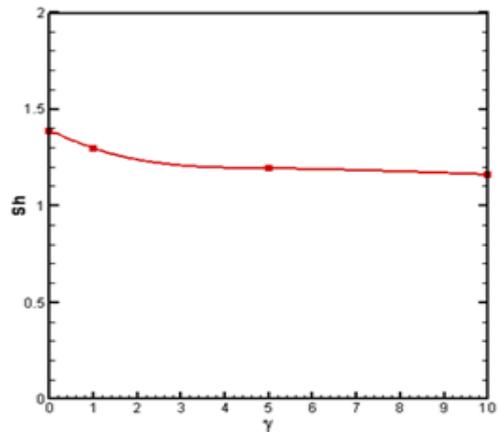


Fig-7(b). Effect of γ on mass transfer with $K = 1$

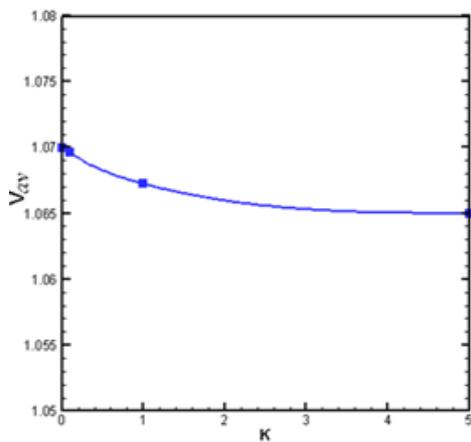


Fig-8(a). Effect of K on average velocity with $\gamma = 5$

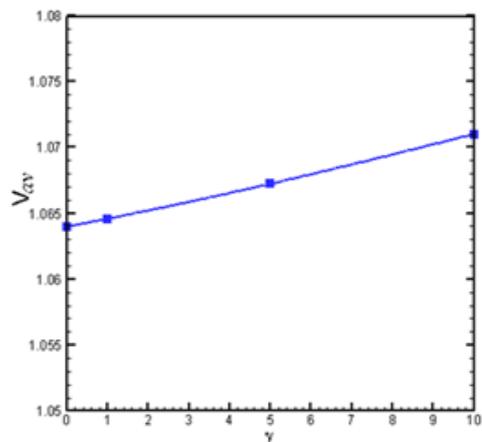


Fig-8(b). Effect of γ on average velocity with $K = 1$

4.5. Effect on Velocity, Temperature and Concentration

The average velocity magnitude V_{av} , temperature Θ_{av} and concentration C_{av} in the domain of the reactor are presented in Figs. 8 (a)-(b) and Figs. 9 (a)-(b). It is observed that the average

velocity increases due to the increase in the heat generation while it decreases for rising chemical reaction. Average temperature and concentration rises for higher values of K as well as γ . The values of mean temperature are lower than that of concentration which indicates temperature gradient is higher than the concentration gradient. This agrees with the phenomena displayed in Figs. 6(a)-(b) and 7(a)-(b).

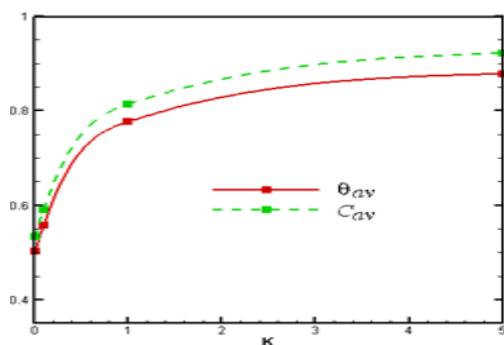


Fig-9(a). Effect of K on average temperature and concentration with $\gamma = 5$

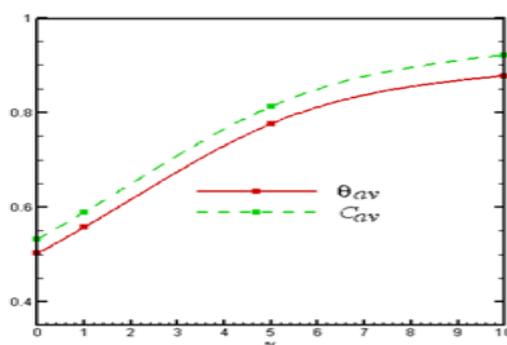


Fig-9(b). Effect of γ on average temperature and concentration with $K = 1$

5. CONCLUSION

Laminar double-diffusive mixed convection flow in a parallel plate reactor with four heated cylinders has been studied for various chemical reactions and heat generation. The following major conclusions are drawn:

- Increment of both K and γ has significant effects on flow, temperature and concentrations.
- Lower temperature and concentration gradient are observed for higher K as well as γ .
- Both heat and mass transfer reduced for rising values of both the parameters.
- Reduced and enhanced velocity is observed according to increasing K and γ respectively.
- The heater placed near the inlet and outlet gives respectively the highest and lowest heat transfer rate.

In general the chemical reaction and heat generation may be the controlling parameters for the heat and mass transfer enhancement in such type of reactor.

Nomenclature

α	thermal diffusivity
β	expansion coefficient
ν	kinematic viscosity
ρ	density
θ	nondimensional temperature
ψ	streamfunction
C	nondimensional concentration

c	concentration
D	mass diffusivity
g	gravitational acceleration
Gr	Grashof number
H	height of the reactor
K	Chemical reaction parameter
L	length of the reactor
Le	Lewis number
N	buoyancy ratio
n	outward normal direction
Nu	average Nusselt number
P	nondimensional pressure
Pr	Prandtl number
Re	Reynolds number
Ri	Richardson number
Sh	average Sherwood number
T	temperature
U, V	nondimensional velocity components
u, v	velocity components
X, Y	nondimensional coordinate
x, y	Cartesian coordinate

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