NUMERICAL MODELING OF HEAT AND MASS TRANSFER USING NANOFLUID IN A TUBULAR REACTOR

by

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Candidate's Declaration

It is hereby declared that this thesis or any part of it has not been submitted elsewhere for the award of any degree or diploma.

Sadikul Islam

This work is dedicated

to

My Mother

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I would like to affirm the continual mercy, help and blessing showered by the Almighty without which it would have been impossible to accomplish the arduous job I was assigned to.

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Abstract

Chemical reactions occur everywhere in our everyday life, for example, in the human body, in cell phone batteries, in a rocket engine and in the pharmaceutical and chemical industry. Optimizing chemical reactors, filtration equipment, mixers, and other processes is made easy with the chemical reaction engineering.

In this research the model provides a study of an elementary, exothermic, 2nd-order reversible reaction in a tubular reactor (liquid phase, laminar flow regime). The aim of this research is to study numerically the effect of convective heat and mass transfer flow of a viscous fluid in the reactor. Assuming that the variations in angular direction around the central axis are negligible makes it possible to reduce the model to a 2D axisymmetric model. The numerical procedure to solve the governing equations with appropriate boundary conditions will be conducted by finite element formulation based on the Galerkin weighted residual approach. The investigation of forced convection flow, heat and mass transfer phenomena through a tubular reactor is carried. The implications of heat of reaction (H), rate of reaction (R) and solid volume fraction of water-copper nanofluid (ϕ) on the flow structure, heat transfer and mass transfer characteristics are presented. The results are presented in the form of isothermal lines, iso-concentrations and stream function, average Nusselt number and Sherwood number. Present numerical results have also been compared with published result and found good agreement. The rates of forced convective heat transfer and mass transfer enhance 14 and 20%, respectively for rising volume fraction (ϕ) upto 3% with compared to base fluid.

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Nomenclature

A	Pre-exponential factor
c	Concentration of fluid (kg/l)
C_p	Specific heat at constant pressure ($J\ kg^{-1}K^{-1}$)
D	Mass diffusivity (m^2/s)
E_a	Activation energy (kJ/mol)
k	Thermal conductivity of fluid ($Wm^{-1}K^{-1}$)
L	Length of the reactor along z axis (m)
H	Heat of reaction (kJ/mol)
m	Mass flow rate (Kgs^{-1})
Nu	Average Nusselt number
p	Pressure ($kgm^{-1}s^{-2}$)
R	Rate of chemical reaction ($mol/m^3/s$)
R_a	Radius (m)
Sh	Mean Sherwood number
T	Fluid temperature (K)
v_r	Velocity in r-direction (ms^{-1})
v_z	Velocity in z-direction (ms^{-1})

Greek symbols

β	Thermal expansion coefficient (K^{-1})
ϕ	Nanoparticles volume fraction
μ	Dynamic viscosity of the fluid (m^2s^{-1})
v	Kinematic viscosity of the fluid (m^2s^{-1})
ρ	Density of the fluid (kgm^{-3})

Subscripts

f	fluid
h	heated
in	input
nf	nanofluid
s	solid particle

Abbreviation

BE	boundary element
BV	boundary volume
CBC	convective boundary conditions
CFD	computational fluid dynamics
FD	finite difference
FE	finite element
FEA	finite element analysis
FEM	finite element method
FV	finite volume
MRI	Magnetic resonance imaging
2D	two dimensional

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Chapter 1: Introduction

1.1 Introduction

The study of a chemical reaction is of paramount importance in chemical engineering. Combined heat and mass transfer problems inside a chemical reactor are of importance in many processes and have, therefore, received a considerable amount attention in recent years.

1.1.1 Tubular Reactor

Chemical reactor is a vessel in which chemical reactions take place. A combination of vessels is known as a chemical reactor network. Chemical reactors have diverse sizes, shapes, and modes and conditions of operation based on the nature of the reaction system and its behavior as a function of temperature, pressure, catalyst properties, and other factors.

Tubular reactors are used in a variety of industries such as petroleum, petrochemical, polymer, pharmaceutical, waste treatment, especially chemical, alternative energy. Tubular reactors are used in a variety of applications such as carbonylation, dehydrogenation, hydrogenation, hydrocracking, hydroformulation, oxidative decomposition, partial oxidation, polymerization, reforming. Figure 1.1 shows different forms of tubular chemical reactor.

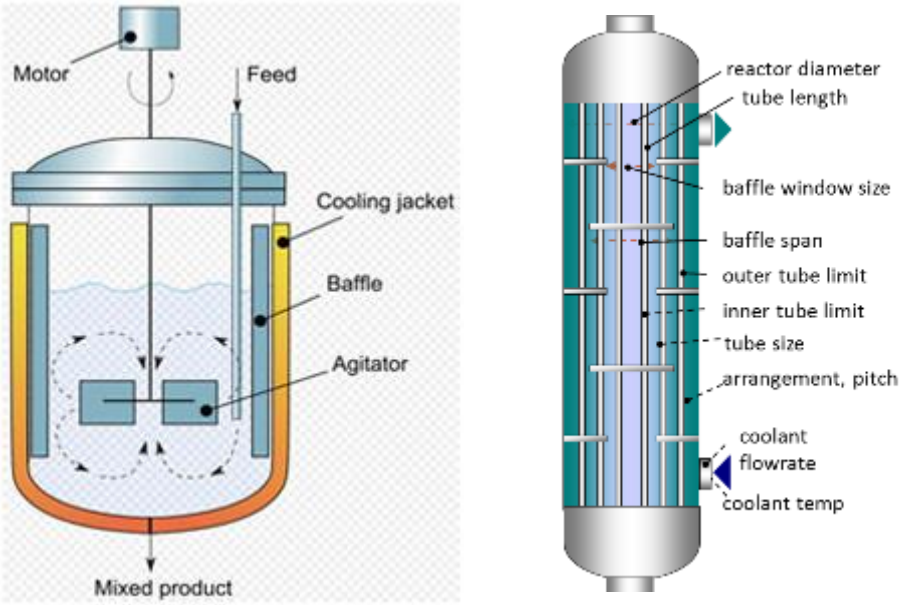

Figure 1.1: Tubular chemical reactors

A tubular reactor is a vessel through which flow is continuous, usually at steady state, and configured so that conversion of the chemicals and other dependent variables are functions of position within the reactor rather than of time. In the ideal tubular reactor, the fluids flow as if they were solid plugs or pistons, and reaction time is the same for all flowing material at any given tube cross section. Tubular reactors resemble batch reactors in providing initially high driving forces, which diminish as the reactions progress down the tubes.

1.1.2 Flow through Tubular Reactor

Flow in tubular reactors can be laminar, as with viscous fluids in small-diameter tubes, and greatly deviate from ideal plug-flow behavior, or turbulent, as with gases. Turbulent flow generally is preferred to laminar flow, because mixing and heat transfer are improved. For slow reactions and especially in small laboratory and pilot-plant reactors, establishing turbulent flow can result in inconveniently long reactors or may require unacceptably high feed rates. Figure 1.2 shows flow through tubular reactor.

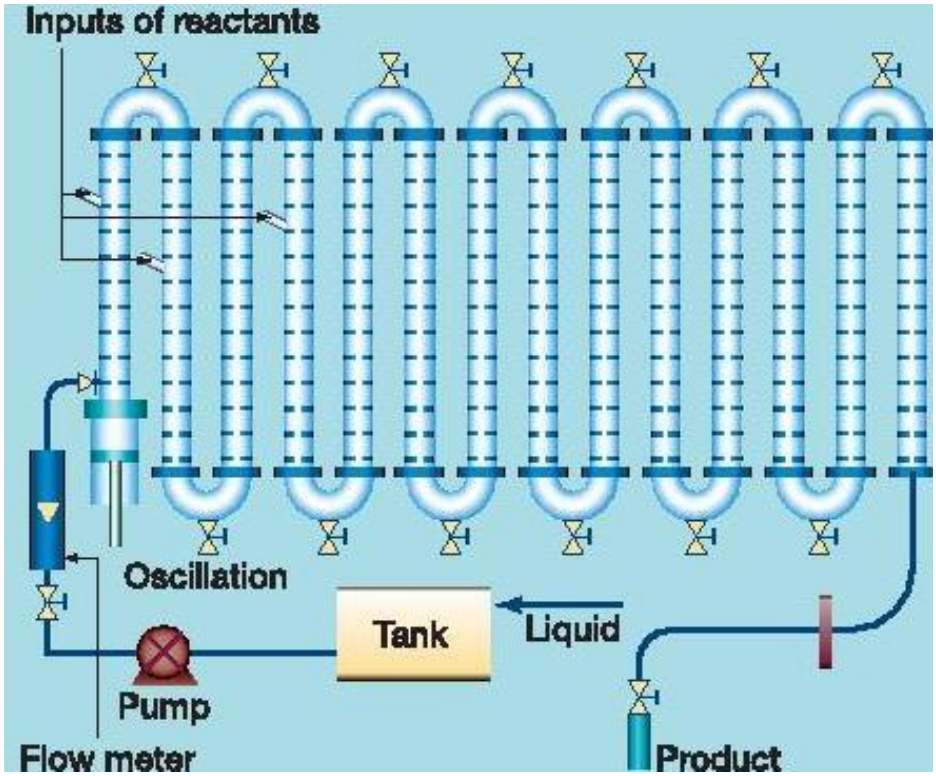

Figure 1.2: Flow through tubular chemical reactor

Flow-through tubular chemical reactor is most widely used for heterogeneous systems. Tubular reactors permit a vigorous heat exchange in the reaction zone and ensure a uniform residence time for all particles in the flow. This reactor is sometimes filled with solid packing in order to accelerate the mass exchange between phases and reduce the variation in residence time of the reactant particles. For reactions involving both a gaseous and liquid phase, a broad surface between the phases is achieved by dispersing one of the reactants. When necessary, flow-through reactors are equipped with circulation loops for recycling any substances that did not react.

1.1.3 Heat and Mass Transfer

Heat and mass transfer problems with chemical reaction are of importance in many processes and have, therefore, received a considerable amount attention in recent years. Heat and mass transfer occur simultaneously in various processes including drying, evaporation at the surface of a water body, energy transfer in a wet cooling tower and the flow in a desert cooler, in chemical reaction engineering etc. Figure 1.3 shows heat and mass transfer.

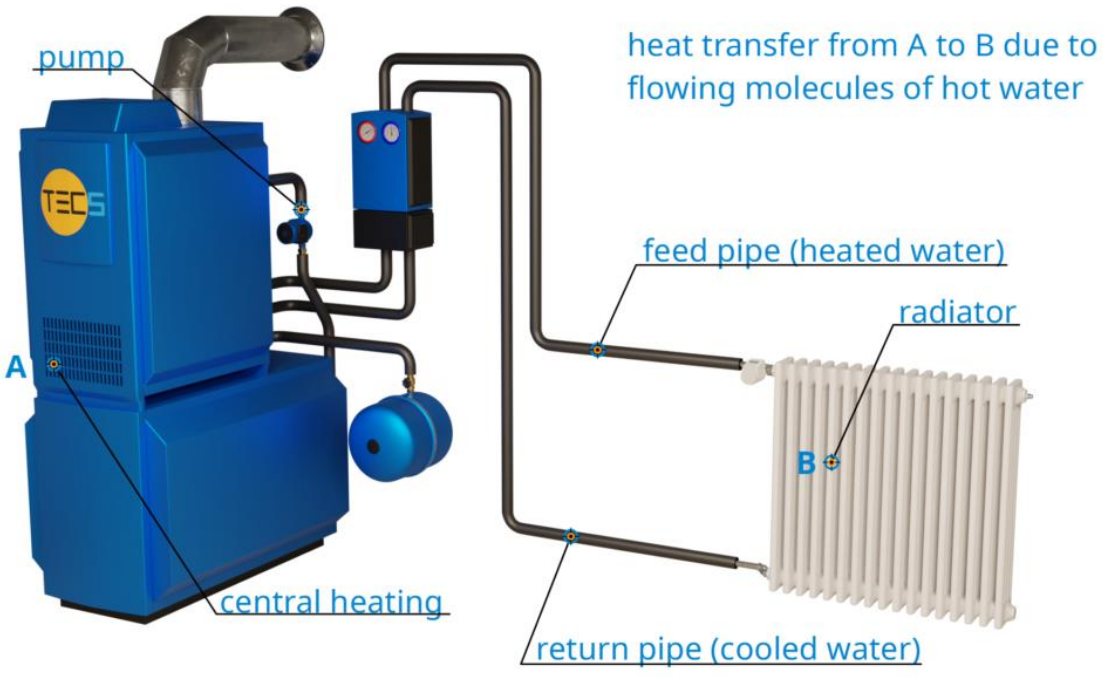

Figure 1.3: Heat and mass transfer

1.1.4 Forced Convection

Forced convection is a mechanism in which fluid motion is generated by an external source (like a pump, fan, suction device etc.). Significant amounts of heat energy can be transported very efficiently by this system and it is found very commonly in everyday life, including central heating, air conditioning, steam turbines and in many other machines. Figure 1.4 shows as forced convection.

Figure 1.4: Forced convection

1.2 Literature Review

Few researchers investigated the effects of forced convective flows in tubular chemical reactor by using analytical, experimental and numerical methods. Some important works are presented below. The assumption of effective or apparent transport parameters is based on the idea of unidirectional axial plug flow of the fluid throughout the reactor. These effective transport parameters are determined empirically, i.e. the parameters lump together all of the contributing physical phenomena. This assumption is still employed frequently in reactor modeling [1-3]. However, this approach has always caused inconsistency in the heat transfer coefficient or wall Nusselt number among a number of reported results. The inconsistency is

originated from the lack of the local-scale flow picture of the bed. Das *et al.* [4] studied the effect of the first order homogeneous chemical reaction on the process of an unsteady flow past an infinite vertical plate with a constant heat and mass transfer. Local heat transfer rates were shown not to be correlated statistically with the local flow field [5]. Steam reforming of hydrocarbons is one of the examples, which is an endothermic reaction [6], while another is CO combustion, which is an exothermic reaction.

Muthucumaraswamy and Ganesan [7] studied effect of the chemical reaction and injection on flow characteristics in an unsteady upward motion of an isothermal plate. The early stage of reactor modeling has been based on simplifying assumption such as homogeneity, effective transport parameters, and pellet effectiveness factors [8]. Homogeneity stands for viewing the fixed-bed as a single phase continuum. The design of catalyst particles for fixed-bed reactor is optimized by computational fluid dynamics (CFD). The CFD is used to obtain detailed flow and temperature fields in the reactor. In the field of reactor engineering, physical demands such as low pressure drop or high heat transfer efficiency are often in conflict with chemical demands such as gas contact efficiency [9]. Heat and mass transport in tubular packed reactors at reacting and non-reacting conditions was analyzed by Koning [10] where the most common models of wall-cooled tubular packed bed reactors were presented. Low tube-to-particle diameter ratio is needed for heat management, i.e. sufficient heat supply from the reactor wall for highly endothermic reaction or sufficient heat removal to the reactor wall for highly exothermic reaction [11].

Recent magnetic resonance imaging (MRI) [12] have demonstrated that heat is transferred not solely by axial flow but also by strong radial convective flows as fluid is displaced around the packing elements. Computational techniques for fluid flow have recently employed for reactor modeling as an alternative method to the semi-empirical method, in attempting to understand detailed flow in the pore scale. The approach was validated by comparing apparent transport parameters with those from model-matching theory based on experimental measurements [13]. Chamkha [14] studied the MHD flow of a numerical of uniformly stretched vertical permeable surface in the presence of heat generation/absorption and a chemical reaction. He assumed that the plate is embedded in a uniform porous medium and moves with a constant velocity in the flow direction in the presence of a transverse

magnetic field. Catalyst design by CFD for heat transfer and reaction in steam reforming was conducted by Nijemeisland *et al.* [15].

Combined heat and mass transfer from a horizontal channel with an open cavity heated from below is numerically examined Brown and Lai [16]. One of the outcomes of CFD is a complex picture of strong radial flow. The pressure and the wall temperature were found to have little or no influence on the apparent heat transfer parameters [17]. Masoumi *et al.* [18] developed a 1D steady-state model for tubular reactors in naphtha cracking. A free-radical reaction scheme including 90 species and 543 reactions was used. An optimization study was performed with the aim to maximize operating. Heat and mass transfer in tubular reactor is shown in [19]. 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. One of the concerns in CFD is that all elements have a finite dimension in all edges, which does not allow actual contact points between solid parts. This limitation causes inconsistency of heat transfer coefficient with the one calculated by model-matching theory. To avoid this, the diameter of the particles was slightly reduced in the model and finer mesh density was applied to wall-particle and particle-particle contact regions [20-21].

Ibrahim *et al.* [22] studied 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. Heat and mass transfer in fixed-bed tubular reactor was analyzed by Kugai [23]. Kesavaiah *et al.* [24] investigated the effect of the chemical reaction and radiation absorption on an unsteady MHD convective heat and mass transfer flow past a semi-infinite vertical permeable moving plate embedded in a porous medium with heat source and suction. 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. Very recently, Parvin *et al.* [25] analyzed numerically the effect of double-diffusive natural convection of a water–Al_2O_3 nanofluid in a partially heated enclosure with Soret and Dufour coefficients. Chemical reaction with heat and mass transfer in chemical reactor is analyzed by Parvin *et al.* [26-28]. Semi-empirical relation for forced convective analysis through a solar collector was studied by Nasrin and Alim [29].

1.3 Objectives

The overall goal of this research project is to numerically simulate fluid flow, heat and mass transfer behaviors through the tubular chemical reactor as stated in previous section. The investigation is to be carried out at heat of reaction and rate of reaction and solid volume fraction of water-Cu nanofluid. Results are presented in terms of isothermal lines, stream function and iso-concentrations as well as the average Nusselt and Sherwood numbers through tubular reactor. However, the specific aims of the study are as follows:

- To solve the mathematical model of tubular reactor numerically.
- To carry out the validation of the present numerical model by investigating the effect of forced convection flow through a tubular reactor.
- To examine the heat and mass transfer characteristics through the reactor for heat of reaction, rate of reaction and volume fraction of nanofluid.

1.4 Scope of Thesis

A brief description of the present numerical investigation of heat transfer inside a wavy trapezoidal enclosure using tubular reactor have been presented in this thesis through five chapters as stated below:

Chapter 1 contains introduction with the aim and objectives of the present work. This chapter also includes a literature review of the discussions, it is seen that there has been a good number of works in the field of heat and mass transfer system through tubular reactor. Objectives of the present study have also been incorporated in this chapter.

There are different numerical methods which include in the Chapter 2 (e.g., Finite difference method, FDM), integral methods (variation and weighted residuals, e.g., FEM), and stochastic methods (e.g., Monte carlo method) description for the numerical simulation of heat transfer as well as nanofluids. In addition, meshing, grid sensitivity test have been illustrated in this chapter.

In Chapter 3 physical model of tubular reactor has been described. The effects of the rate of reaction (R), heat of reaction (H) and volume fraction (ϕ) of water copper on heat-mass

transfer, fluid velocity through the tubular reactor have been studied. The comparison of present numerical result with that of Kugai [23] has been shown as well as percentage of error has been calculated.

Chapter 4 concludes remarks of the whole research and the recommendations for the future research.

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Chapter 2: Numerical Techniques

2.1 Introduction

Physical phenomena may be described mathematically by ordinary or partial differential equations, which are the subject matter of analytical and numerical investigations. The partial differential equations concerning fluid mechanics, heat and mass transfer may be solved analytically only for a limited number of cases. With the help of computer, approximate solution may be obtained numerically where the differential equations are approximated by a system of algebraic equations using discretization technique. The solution domain is discretized into small sub-domains where the numerical solutions give results at discrete locations in space and time. The accuracy of numerical results depends on the accuracy of available experimental data and the quality of discretizations used.

Computational fluid dynamics (CFD) is a branch of fluid mechanics that uses numerical methods and algorithms to solve and analyze problems of fluid flows. Computers are used to perform the calculations required to simulate the interaction of liquids and gases with surfaces defined by boundary conditions. With high-speed supercomputers, better solutions can be achieved. Engineers use CFD codes that can make physically realistic results with high accuracy in simulations using finite grids. Contained within the broad field of computational fluid dynamics are activities that cover the range from the automation of well established engineering design methods to the use of detailed solutions of the Navier-Stokes equations as substitutes for experimental research into the nature of complex flows. CFD have been used for solving wide range of fluid dynamics problem. It is most frequently used in fields of engineering where the geometry is complicated or some important feature that cannot be dealt with other methods.

2.2 Advantages of Numerical Analysis

The problems of fluid flow, heat and mass transfer may be analyzed either theoretically or experimentally. From the economical point of view, experimental investigation of such problems could not draw much attention because of their inadequate flexibility and

applications. However, often experimental investigation is necessary to validate numerical method. Separate experimental arrangement/ set up requires for any change in the geometry

and boundary condition of the systems for their investigation. Time involvement is also a factor to make it unappealing. On the other hand, the theoretical analysis can be carried out either by analytical approach or by numerical approach. In solving the practical problems, the analytical solution methods are not of much popular. Numerical methods are extremely powerful problem-solving tools that are capable of handling large systems of equation, complicated geometries etc., which is often impossible to solve analytically. General closed form solutions can be obtained only for very ideal cases and the results obtained for a particular problem, usually with uniform boundary conditions. For two-dimensional thermodynamic problems, mathematical model involve partial differential equations that are required to be solved simultaneously with some boundary conditions. Therefore, numerical methods are the easier way to find out solutions of the problems of practical interest because it reduces higher mathematics to basic arithmetic operations.

2.3 Major Steps of a Numerical Solution

The main steps from various components of numerical solution are as follows:

2.3.1 Mathematical model

The starting point of any numerical method is to develop a mathematical model which consists of a set of partial differential equations or integro-differential equations and boundary conditions. A solution method is usually designed for a particular set of equations. A general-purpose solution method, i.e. one which is applicable to all flows, is impractical, though not impossible and with most general purpose tools, they are usually not optimum for any single application.

2.3.2 Discretization technique

After selecting the mathematical model, one has to choose a suitable discretization method, i.e. a method of approximating the differential equations by a system of algebraic equations for the variable at some set of discrete locations in space and time. There are several

approaches, the most important of which are: finite difference (FD), finite volume (FV) and finite element (FE) methods.

2.3.3 Mesh

The discrete locations at which the variables are to be calculated are defined by a mesh which covers the geometric domain on which the problem is to be solved. It divides the solution domain into a finite number of sub-domains called finite elements, control volumes, etc.

2.3.4 Accuracy

Numerical solutions of physical event are only approximate solutions. Numerical solutions usually incorporate three kinds of systematic errors.

- Modeling errors which occur due to the difference between the actual physical phenomena and the exact solution of the mathematical model.
- Discretization errors, defined as the dissimilarity between the exact solution of the equation of the model and the exact solution of that algebraic system of equations obtained by discretizing these equations and
- Iteration errors, defined as the difference between the iterative and exact solutions of the algebraic systems of equations.

It is important to identify these errors, and distinguish them. Various errors may cancel each other, so that sometimes a solution obtained on a coarse mesh, pretends to agree better with the experiment than a solution on a finer mesh, which should be more accurate. Therefore, meshing has to be dealt with very carefully.

2.3.5 Solution method

Practical applications of the finite element method lead to large systems of simultaneous linear algebraic equations. Fortunately, finite element equation systems possess some properties which allow reducing storage and computing time. The finite element equation systems are: symmetric, positive definite and sparse. Symmetry allows storing only half of the matrix including diagonal entries. Positive definite matrices are characterized by large positive entries on the main diagonal. Solution can be carried out without pivoting. A sparse matrix contains more zero entries than nonzero entries. Sparsity can be used to economize

storage and computations. Solution methods for linear equation systems can be divided into two large groups: direct methods and iterative methods. Direct solution methods are usually used for problems of moderate size. For large problems iterative methods require less computing time and hence they are preferable. The choice of solver depends on the grid type and the number of nodes involved in each algebraic equation.

2.4 Finite Element Modeling: Implementation and Solution

The solution of the heat and mass transfer model equations (presented in chapters 3 and 4) provides the predictions of state variables (e.g. velocity, temperature, concentration) in space and time. The solutions of coupled partial differential equations (PDE) require the numerical method. The FEM, is used to solve the model equations of heat and mass transfer. The FEM solution provides a quantitative understanding of heat and mass transfer.

2.4.1 Numerical solution

Discretization is the first step to solve numerically a mathematical model of physical phenomena. That is, the differential equations are transformed into a "numerical analogue" which can be represented in the computer and then processed by a computer program built on some algorithm. There are many discretization schemes such as finite difference (FD), finite volume (FV), finite element (FE) methods, Boundary element (BE) method and Boundary volume (BV) method. The present numerical computation has been performed by finite element method (FEM). Detailed analysis of this method is available in Chung [30] and Dechaumphai [31].

In the past few years the growth of powerful computers with greater computational capabilities has facilitated the formulation of sophisticated numerical methods that simulate the real physical systems by solving complex mathematical models (Moens and Vandepitte [32], Mohamed [33], Wang and Sun [34]). In the literature, there are different numerical methods which include differential methods (e.g., Finite difference method, FDM), integral methods (variation and weighted residuals, e.g., FEM), and stochastic methods (e.g. Monte Carlo method) (Sandeep *et al.* [35]). In engineering applications, the FDM and the FEM are the commonly employed numerical techniques. The former is a less complex and computationally inexpensive method compared to the latter (Wang and Sun [34]). However,

the latter has several advantages compared to the former the FEM is more flexible in handling the spatial variation of material properties, irregular shape and regions, nonlinear problem, mixed boundary and initial conditions. Therefore, FEM was chosen to solve the mathematical model of coupled heat and mass transfer.

2.4.2 Finite Element method

The finite element discretization divides the problem domain of interest into a finite number of elements, and each element is connected to each other at points called nodes (Sandeep *et al.* [35]). The collection of the elements and nodes is called the Finite Element mesh (figure 2.1). The nodes typically lie on the element boundary where adjacent elements are connected. The nodal values of the field variable and the interpolating functions for the elements define the behavior of the field variable within the elements. The nodal points depict the field variable or the unknown, defined in terms of approximating or interpolating functions within each element. A detailed discussion of the FEM and techniques can be found in many books, for example Martins *et al.* [36], Puri and Anantheswaran [37].

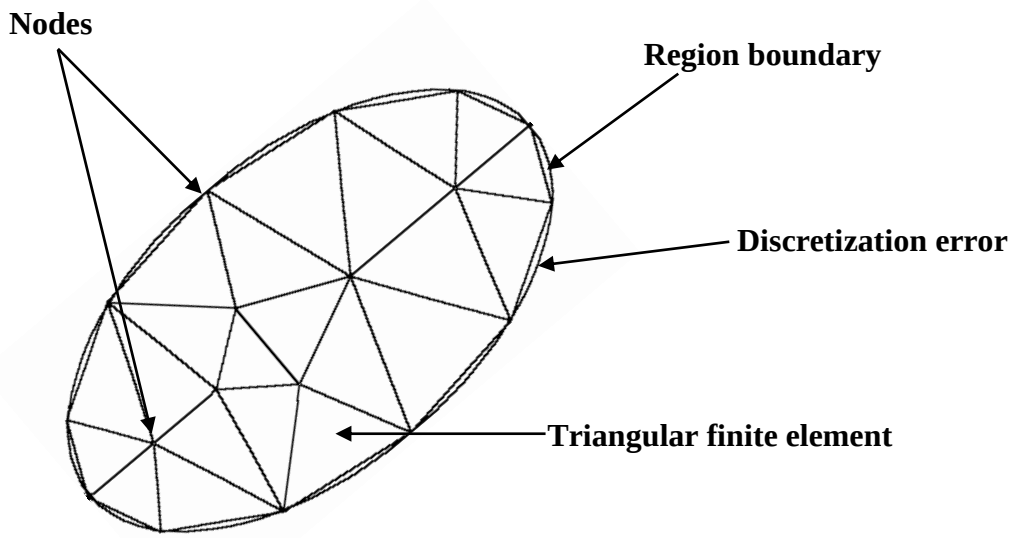


Figure 2.1: Two dimensional finite element mesh

Chapter 3: Forced Convective Nanofluid Flow through Tubular Reactor

3.1 Introduction

The reactors, in which chemicals are made in industry, vary in size from a few cm^3 to the vast structures that are often depicted in photographs of industrial plants. In a tubular reactor, fluids (gases and/or liquids) flow through it at high velocities. As the reactants flow, for example along a heated pipe, they are converted to products. At these high velocities, the products are unable to diffuse back and there is little or no back mixing. The conditions are referred to as plug flow. This reduces the occurrence of side reactions and increases the yield of the desired product. Tubular reactors are used, for example, in the steam cracking of ethane, propane and butane and naphtha to produce alkenes.

In this chapter, the study addresses the assisted (forced) convective flow, heat and mass transfer phenomena through a tubular chemical reactor. Numerical solutions has been obtained over a wide range of rate of reaction (R), heat of reaction (H) and solid concentration (ϕ) of water copper nanofluid. The numerical results have been presented graphically in terms of isothermal lines, streamlines, iso-concentrations. Finally, the rate of heat transfer (Nu) and mass transfer (Sh) have been calculated.

3.2 Physical Configuration

The model geometry of tubular reactor is given in figure 3.1. This model consists of an inlet boundary, an outlet boundary, a reactor wall facing the cooling jacket, a cooling jacket, and a symmetry line running axially along the tubular reactor.

Assuming that the variations in angular direction around the central axis are negligible makes it possible to reduce the model to a 2D axisymmetric model. A schematic diagram of the system considered in the present research is shown in figure 3.2. In this study, an axial two dimensional tubular reactor model is built up numerically using software. L and R_a are the length and radius of the reactor. Only steady state case is considered.

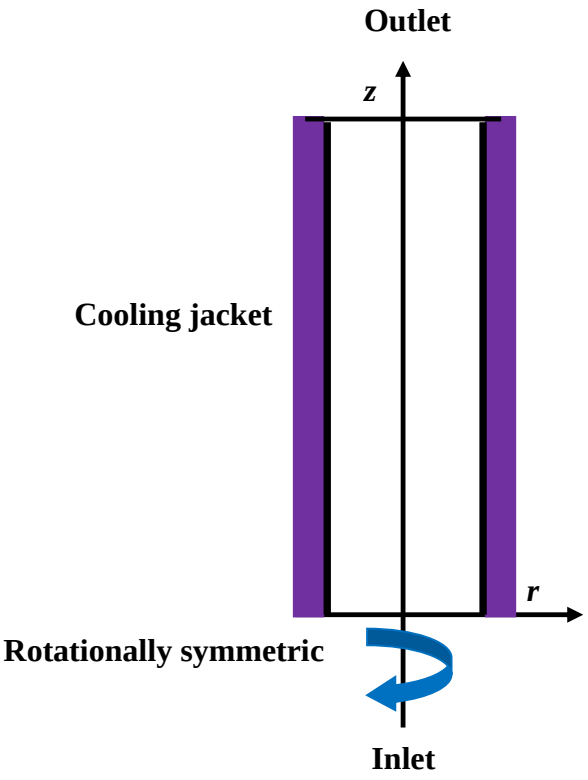


Figure 3.1: 2D rotationally symmetric model of tubular reactor

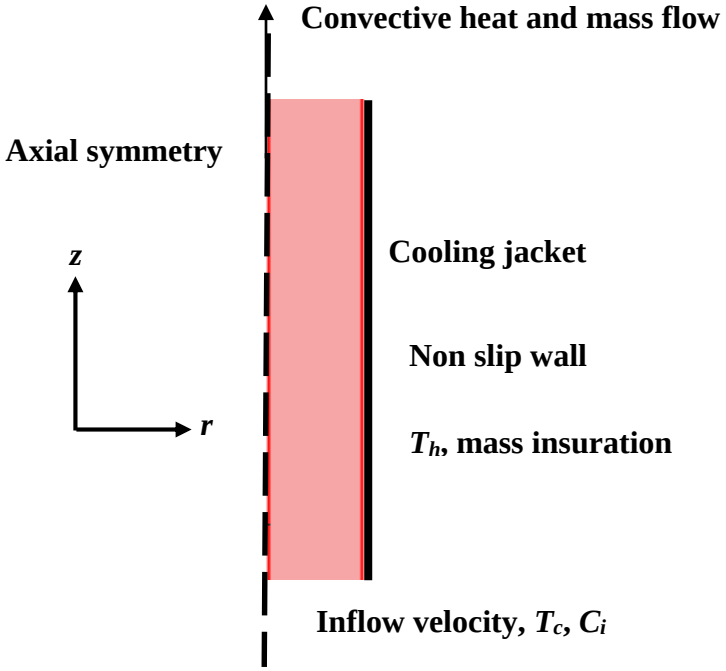


Figure 3.2: Schematic diagram of the tubular reactor

3.3 Mathematical Formulation

The reactor is equipped with a cooling jacket to limit the temperature increase due to the exothermic nature of the reaction and avoid an explosion. Under the assumptions that the coolant flow mixing eliminates any temperature differences in the radial direction, only axial temperature variations are present in the cooling jacket. The contribution of heat conduction in the cooling jacket is neglected and thus it is assumed that heat transport takes place only through convection. For this reason, the cooling jacket is not included in the model geometry.

The mass, momentum, energy and material balances for the tubular reactor can be described according to Kugai [23] and given as follows:

Mass Conservation Equation:

$$\frac{1}{r}\frac{\partial(rv_r)}{\partial r}+\frac{\partial(v_z)}{\partial z}=0 \tag{3.1}$$

Momentum Conservation Equations:

$$\rho_{nf}\left\{\frac{1}{r}\frac{\partial}{\partial r}(rv_rv_r)+\frac{\partial}{\partial z}(rv_zv_r)\right\}=-\frac{\partial p}{\partial r}+\mu_{nf}\left\{\frac{2}{r}\frac{\partial}{\partial r}\left(r\frac{\partial v_r}{\partial r}\right)+\frac{\partial}{\partial z}\left(r\frac{\partial v_r}{\partial z}\right)-2\frac{v_r}{r^2}+\frac{\partial}{\partial z}\left(\frac{\partial v_z}{\partial r}\right)\right\} \tag{3.2}$$

$$\rho_{nf}\left\{\frac{1}{r}\frac{\partial}{\partial r}(rv_rv_z)+\frac{\partial}{\partial z}(rv_zv_z)\right\}=-\frac{\partial p}{\partial z}+(\rho\beta)_{nf}g\beta(T-c)+$$
$$\mu_{nf}\left\{\frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial v_z}{\partial r}\right)+2\frac{\partial}{\partial z}\left(\frac{\partial v_z}{\partial z}\right)+\frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial v_r}{\partial z}\right)\right\} \tag{3.3}$$

Energy Conservation Equation:

$$\left(\rho C_p\right)_{nf}\left\{v_r\frac{\partial T}{\partial r}+v_z\frac{\partial T}{\partial z}\right\}=k_{nf}\left\{\frac{\partial}{\partial z}\left(\frac{\partial T}{\partial z}\right)+\frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial T}{\partial r}\right)\right\}+\left(\sum_j-\Delta H_{r,j}\right)\left(Ae^{\frac{-E_a}{G_cT}}\right) \tag{3.4}$$

Material Conservation Equation:

$$\left(\rho C_p\right)_{nf}\left\{v_r\frac{\partial c}{\partial r}+v_z\frac{\partial c}{\partial z}\right\}=D_{nf}\left\{\frac{\partial}{\partial z}\left(\frac{\partial c}{\partial z}\right)+\frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial c}{\partial r}\right)\right\}-Ae^{-\left(\frac{E_a}{G_cT}\right)} \tag{3.5}$$

Here the effective density $\rho_{nf}=(1-\varphi)\rho_f+\varphi\rho_s$,

the effective heat capacitance $\left(\rho C_p\right)_{nf}=(1-\phi)\left(\rho C_p\right)_f+\phi\left(\rho C_p\right)_s$,

the effective dynamic viscosity of Brinkman model [38] $\mu_{nf} = \mu_f \left(1-\phi\right)^{-2.5}$,

and the effective thermal conductivity of Maxwell Garnett (MG) model [39] $k_{nf} = k_f \dfrac{k_s + 2k_f - 2\phi\left(k_f - k_s\right)}{k_s + 2k_f + \phi\left(k_f - k_s\right)}$,

the effective specific heat at constant pressure $C_{Pnf} = \frac{(1-\phi)(\rho Cp)_f + \phi(\rho C_P)_s}{(1-\phi)\rho_f + \phi\rho_s}$,

The effective thermal diffusivity $(\rho\beta)_{nf} = (1-\varphi)(\rho\beta)_f + \varphi(\rho\beta)_s$

the effective mass diffusivity $D_{nf} = D_f(1-\phi)$

the rate of reaction $R = -A\exp\left(-\dfrac{E_a}{G_c T}\right)$,

and the heat of reaction $H = \left(\sum_j -\Delta H_{r,j}\right)\left(Ae^{\frac{-E_a}{G_c T}}\right)$.

The boundary condition also simulated the actual reaction condition. Figure 3.2 shows the boundary conditions for velocity, temperature, and concentration. The fluid velocity at inlet is assumed laminar flow with average velocity of 0.085 m/s, temperature of 323 K and concentration of 2.542 mol/m^3.

The boundary conditions are:

at the inlet: $v_r = 0$, $v_z = v_{in}$, $T = T_{in}$, $c = C_{in}$

at the outlet: convective heat and mass boundary condition

at the right wall: non slip condition, $T = T_h = 473$ K, mass insuration condition

at the left wall: axial symmetry condition.

The inlet gas composition: 13% CO - 8% CO_2 - 28% H_2O - 51% H_2

Water gas shift reaction: $CO + H_2O = CO_2 + H_2$

The gas composition corresponds to 2.542 mol/m^3 of CO concentration. The effect of water gas shift reaction is included in heat and mass transfer. However, the fluid is assumed to be

ideal gas, so that the equation of momentum balance is independent of those of heat and mass transfer. The heat capacity is similar for four gas components, suggesting convective heat flux is not so much affected by change of gas composition during reaction. Thermal conductivity is more influenced since H_2 has 5 to 10 times of thermal conductivity than the other gases, but the difference becomes smaller in high temperature. Therefore, these parameters were assumed independent of gas composition and water gas shift reaction throughout the reactor. The pressure drop is negligible, so pressure applied at outlet does not influence on the velocity field.

3.3.1 Average Nusselt and Sherwood numbers

The average Nusselt number (*Nu*) and average Sherwood number (Sh) are expected to depend on a number of factors such as thermal conductivity, heat capacitance, viscosity, and flow structure. According to [26-28] the rate of heat transfer along the right heated wall of the tubular reactor may be written as $Nu = \frac{-1}{L}\frac{k_{n_f}}{k_f}\int_0^L \frac{\partial T}{\partial r}\,dz$

and the rate of mass transfer along the inlet opening as $Sh = -\frac{1}{R_a}\frac{D_{nf}}{D_f}\int_0^{R_a} \frac{\partial c}{\partial z}\,dr$

3.3.2 Thermo-physical Properties

The thermo-physical properties of the water, nanoparticle, different gases at 323 K are taken from [40-42] and given in Table 3.1.

Table 3.1: Thermo physical properties of fluid and nanoparticle

Characteristics	**Water**	**Cu**	**CO**	**CO_2**	**H_2**
C_p (J $kg^{-1}K^{-1}$)	4179	385	1050	834	14300
K ($Wm^{-1}K^{-1}$)	0.6	401	0.027	0.018	0.196
ρ (kgm^{-3})	988	8933	1478	2337	106
D (m^2s^{-1})	0.0000242	0.000120	0.0000205	0.0000151	0.0000840

3.4 Computational Procedure

The governing equations along with the boundary conditions are solved numerically, employing Galerkin weighted residual finite element techniques. To derive the finite element equations, the method of weighted residuals [43-44] is applied to the governing equations (3.1) – (3.5). The six node triangular element is used in this work for the development of the finite element equations. All six nodes are associated with velocities, temperature as well as concentration. Only the corner nodes are associated with pressure. This means that a lower order polynomial is chosen for pressure and which is satisfied through continuity equation. Gauss's Divergence theorem is applied to transfer the 2nd ordered derivative part of the governing equations into 1st order derivatives. Gaussian quadrature technique is used in momentum, energy and concentration equations in order to generate the boundary integral terms associated with the surface tractions, heat flux and concentration flux. The basic unknowns for the above differential equations are the velocity components u_r, u_z, the temperature T, the concentration c and the pressure p. These element matrices are evaluated in closed form ready for numerical simulation. Substituting the element velocity components, the temperature, the concentration and the pressure distributions to the governing equations the linear algebraic equations are obtained. Then the equations are solved by applying the Newton-Raphson iteration technique. This leads to a set of algebraic equations with the incremental unknowns of the element nodal velocity components, temperatures, concentration and pressures. The iteration process is terminated if the percentage of the overall change compared to the previous iteration is less than the specified value. To solve the sets of the global nonlinear algebraic equations in the form of matrix, the Newton-Raphson iteration technique has been adapted through PDE solver. The convergence of solutions is assumed when the relative error for each variable between consecutive iterations is recorded below the convergence criterion ε such that $\left|\Psi^{n+1} - \Psi^{n}\right| < \varepsilon$, where n is number of iteration and $\Psi = v_r, v_z, T, c$ and p. The convergence criterion was set to $\varepsilon = 10^{-6}$.

3.4.1 Grid refinement check

An extensive mesh testing procedure is conducted to guarantee a grid-independent solution for H = 10 kJ/mol, R = 1 mol/m^3/s and solid concentration ϕ = 1% through the tubular

reactor. In the present work, five different non-uniform grid systems are examined with the following number of elements within the resolution field: 86, 270, 906, 2024 and 5896. The numerical scheme is carried out for highly precise key in the *Nu* and *Sh* for the aforesaid elements to develop an understanding of the grid fineness as shown in Table 3.2. The scale of the average Nusselt and Sherwood numbers for 2024 elements shows a little difference with the results obtained for the other elements. Hence, considering the non-uniform grid system of 2024 elements is preferred for the computation.

Table 3.2: Grid test at H = 10 kJ/mol, R = 1 mol/m^3/s and ϕ = 1%

Elements	86	270	906	2024	5896
Nu	6.83	7.24	7.72	8.3	8.304
Sh	0.53	0.71	0.92	1.09	1.0913
Time (s)	58	121	211	296	403

3.4.2 Mesh generation

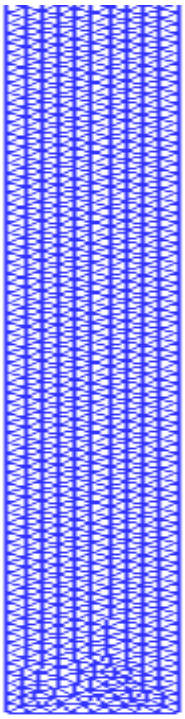


Figure 3.3: Mesh generation of the tubular reactor

In the finite element method, the mesh generation is the technique to subdivide a domain into a set of sub-domains, called finite elements, control volume, etc. The discrete locations are defined by the numerical grid, at which the variables are to be calculated. It is basically a discrete representation of the geometric domain on which the problem is to be solved. The computational domains with irregular geometries by a collection of finite elements make the method a valuable practical tool for the solution of boundary value problems arising in various fields of engineering. Figure 3.3 displays the finite element mesh of the present physical domain.

3.5 Result and Discussions

Finite element simulation is applied to perform the analysis of laminar forced convection temperature, fluid flow, concentration through a tubular chemical reactor. Effects of the rate of reaction (R), heat of reaction (H) and solid concentration (ϕ) of water-copper nanofluid on heat-mass transfer, fluid velocity, thermal and concentration fields through the tubular reactor have been studied. The ranges of H, R and ϕ for this investigation vary from slightly endothermic (- 450 kJ/mol) to highly exothermic (+ 50 kJ/mol), from 1 mol/m^3/s to 7 mol/m^3/s and from 0 to 3%, respectively. The outcomes for the different cases are presented in the following sections:

3.5.1 Effect of heat of reaction (H)

Figure 3.4 (a-c) exhibits the effect of H on the, isotherms, iso-concentrations and streamlines. The values of heat of reaction (H) are - 450 kJ/mol, - 250 kJ/mol, 10 kJ/mol and 50 kJ/mol are chosen to examine the evolution of isotherm, concentration and streamline patterns. Heat of reaction (H) is varied from slightly endothermic (+ 50 kJ/mol) to highly exothermic (- 450 kJ/mol). Here R = 1 mol/m^3/s and ϕ = 1% are kept fixed.

Isothermal lines have significant change due to the variation of H. At H = - 450 kJ/mol, isothermal lines appear at the right hot surface of the tubular reactor. But for higher values of H, these lines spread all over the reactor. It is seen from the figure that, at the highest value of H (+ 50 kJ/mol), the lower temperature lines remain at the inlet portion where as the higher temperature lines at the right surface. Temperature gradient at the heat source becomes lower

for increasing heat generation in the fluid. This happens because higher temperature of the fluid produces lower temperature difference between the hot surface and the fluid.

Iso-concentration lines have also considerable change due to generating heat as shown in figure 3.4(b). Iso-concentration lines spreads all over the tubular chemical reactor. As heat generation increases these lines depart to the exit port which indicates higher mass transportation. This phenomenon is logical because heat generation causes higher velocity which leads to more concentration transfer

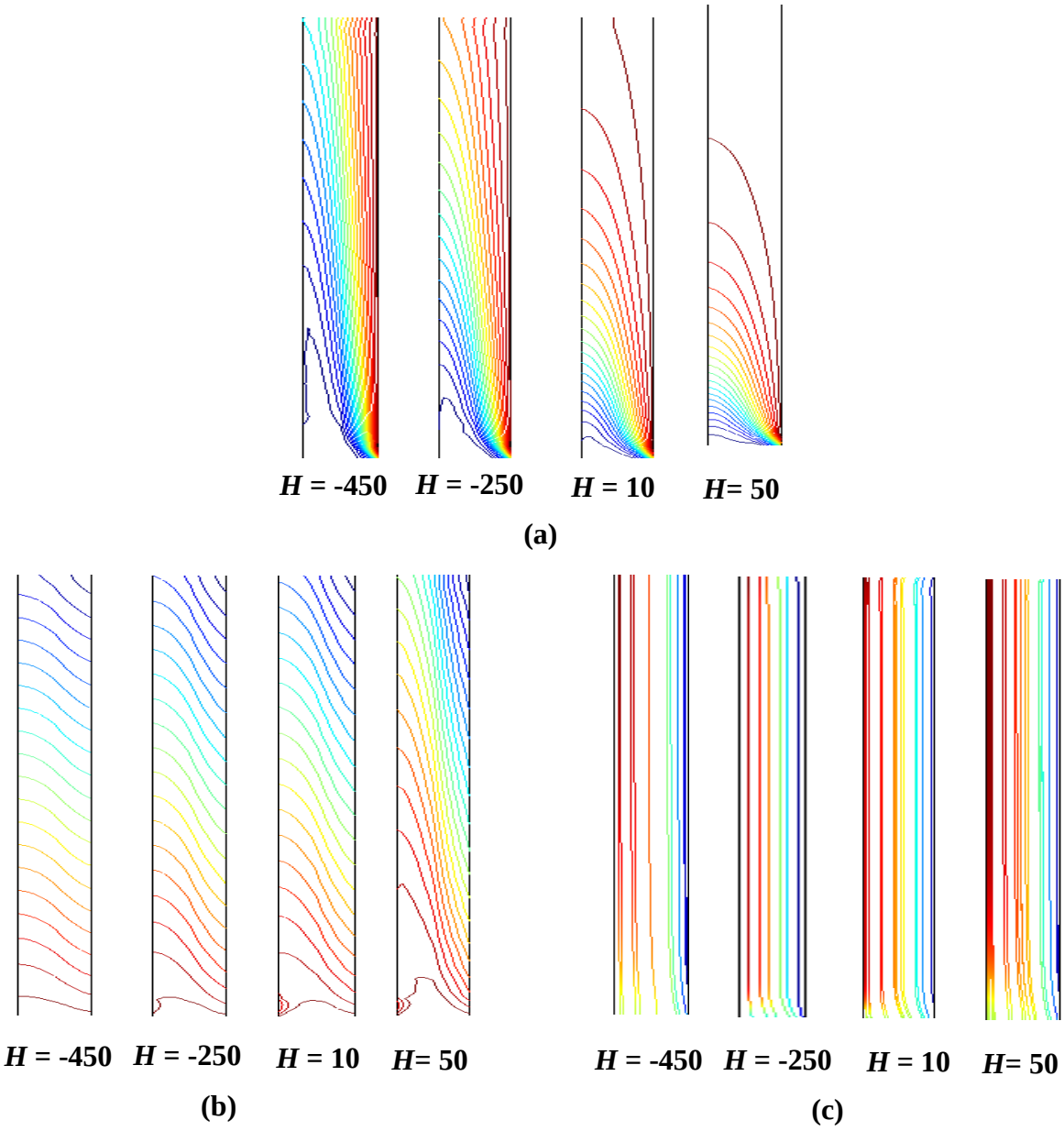
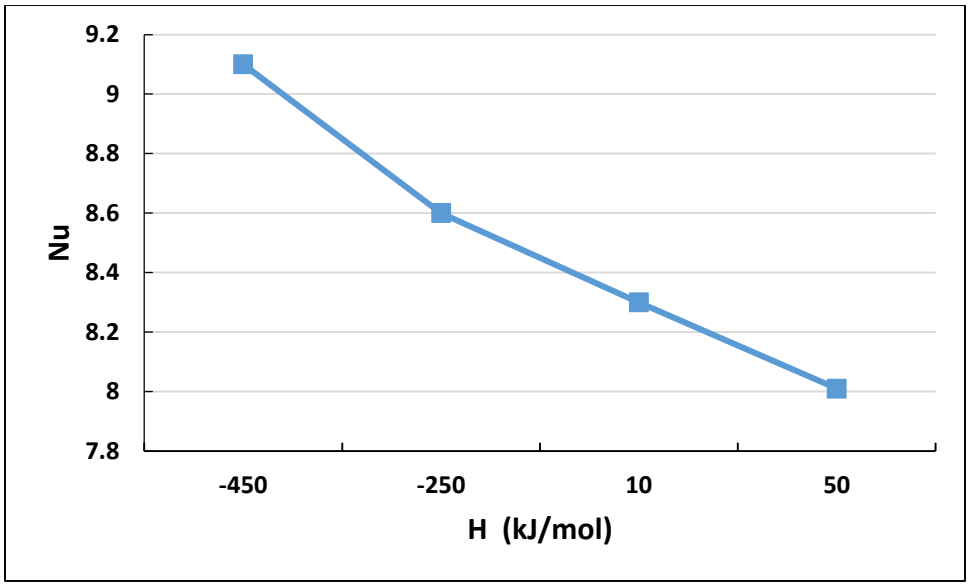
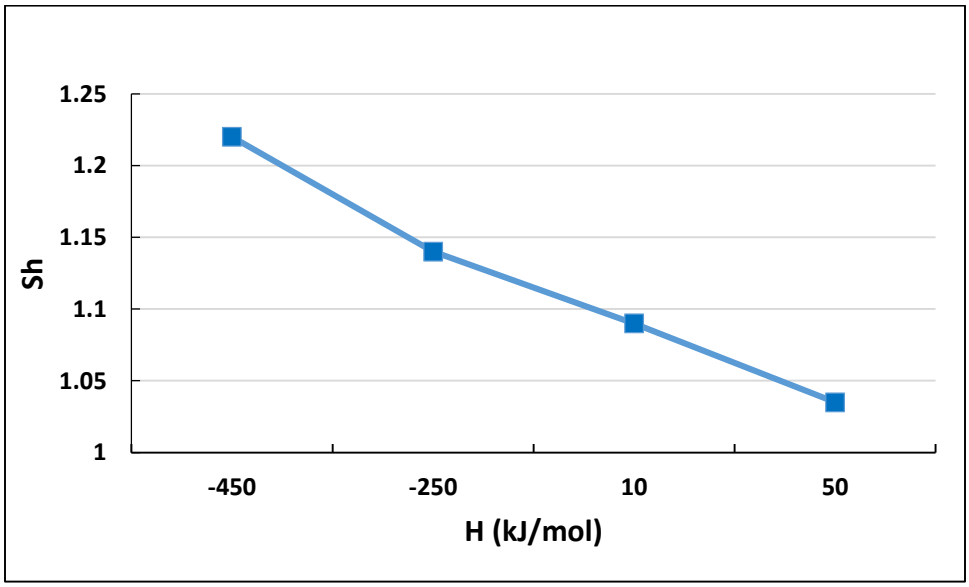


Figure 3.4: Effect of *H* on (a) isotherms, (b) iso-concentrations, and (c) streamlines



(i)



(ii)

Figure 3.5: Effect of *H* on (i) Nusselt number and (ii) Sherwood number

It is observed from figure 3.4(c) that there is a common trend of the development of streamlines with increasing heat generation parameter. The streamlines are almost parallel to the reactor wall and condensed near the right surface and axial symmetric surface. The streamlines become more condensed along the middle of the channel due to increasing heat generation effect. This indicates higher velocity.

The heat and mass transfer rates concentration, magnitude of average sub-domain velocity for fluid with the variation of heat of reaction (*H*) are displayed in figure 3.5(i)- (ii). It is seen from figure 3.5(i) that the highest heat transfer rate is observed for the exothermic flow (*H* = - 450 kJ/mol). Increasing *H* decreases the value of *Nu* due to lowering the temperature difference Enhanced mass transfer rate (*Sh*) is observed in figure 3.5(ii) for decreasing values of heat of reaction (*H*). The rates of forced convective heat and mass transfer decrease by 12 and 15%, respectively for increasing heat of reaction (*H*).

3.5.2 Effect of rate of reaction (*R*)

The effect of rate of chemical reaction (*R*) on the isotherms, iso-concentrations and streamlines is exhibited in figure 3.6 (a-c). In fact, the analysis is performed at forced convection regime by fixing H = 10 kJ/mol and ϕ = 1%. The values of chemical reaction rates are 1, 3, 5 and 7 mol/m^3/s are chosen to examine the evolution of isotherms, iso-concentrations and streamlines patterns.

The isothermal lines have considerable change due to the variation of *R*. 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 rate of chemical reaction, appearance of these lines is more at the outlet opening. It is seen from the figure 3.6(a) that, at the highest value of *R*, the lower temperature lines remain at the inlet opening where as the higher temperature lines at the exit port. Temperature gradient at the right heated surface becomes lower for increasing chemical reaction in the fluid. This happens because higher temperature of the fluid produces lower temperature difference between the heated surface and the fluid.

Figure 3.6(b) shows the iso-concentration lines which have also substantial change due to generating chemical reaction. Iso-concentration lines spreads all over the tubular chemical reactor. As rate of chemical reaction increases, these lines depart to the exit port. Higher concentration causes lower concentration gradient which indicates lower mass transportation.

This phenomenon is logical because generating chemical reaction causes higher velocity which leads to more concentration transfer. The CO concentration distribution showed slightly higher concentration towards the axis, due to high diffusion of mass and/or high reaction rate caused by heat from the wall. There is a common trend of the development of streamlines with generating chemical reaction inside the computational domain. The

streamlines are almost parallel to the channel wall and condensed in axial symmetric region. In addition, the streamlines become more condensed along the middle of the tubular reactor due to increasing chemical reaction effect. This indicates higher velocity.

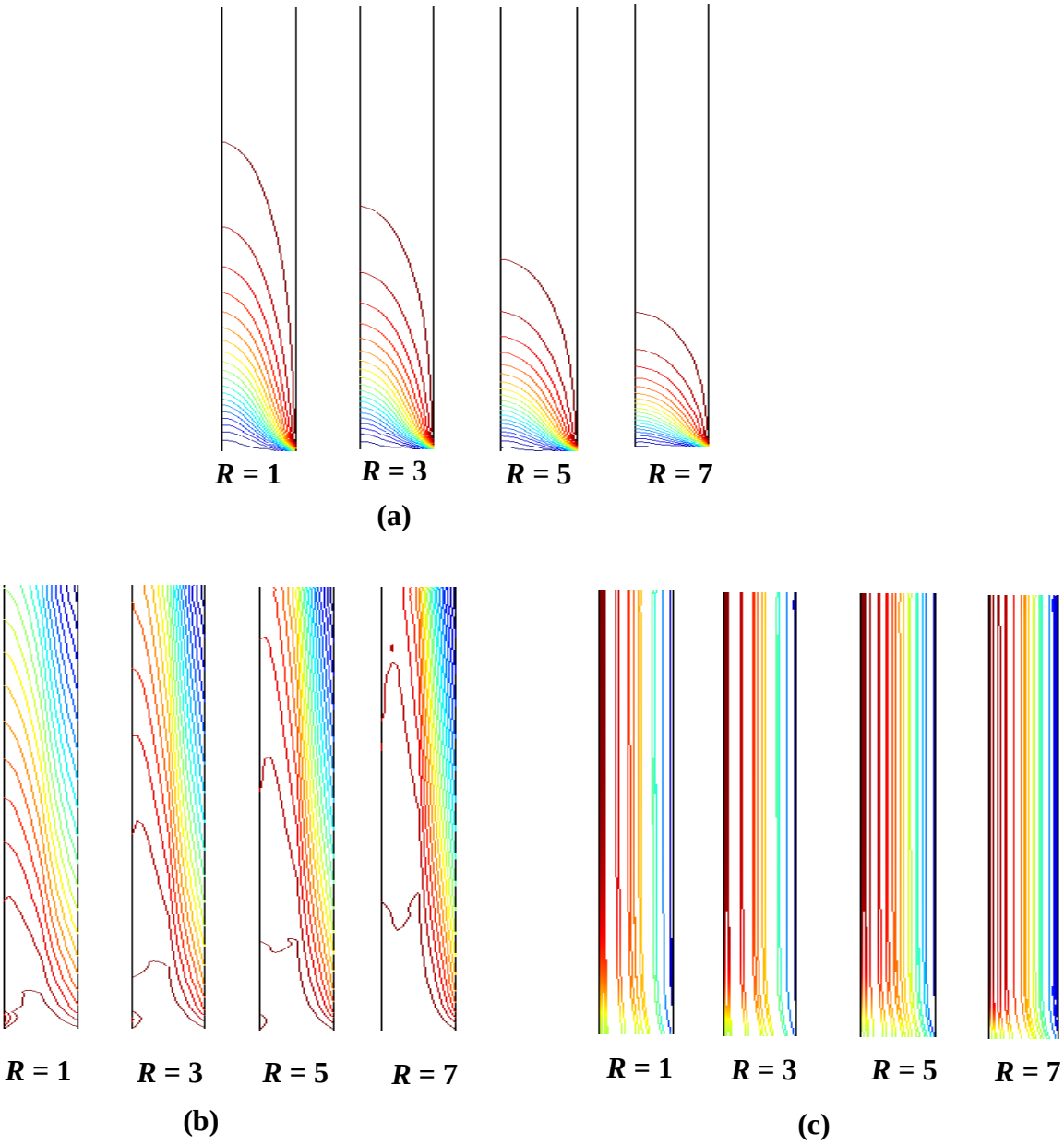
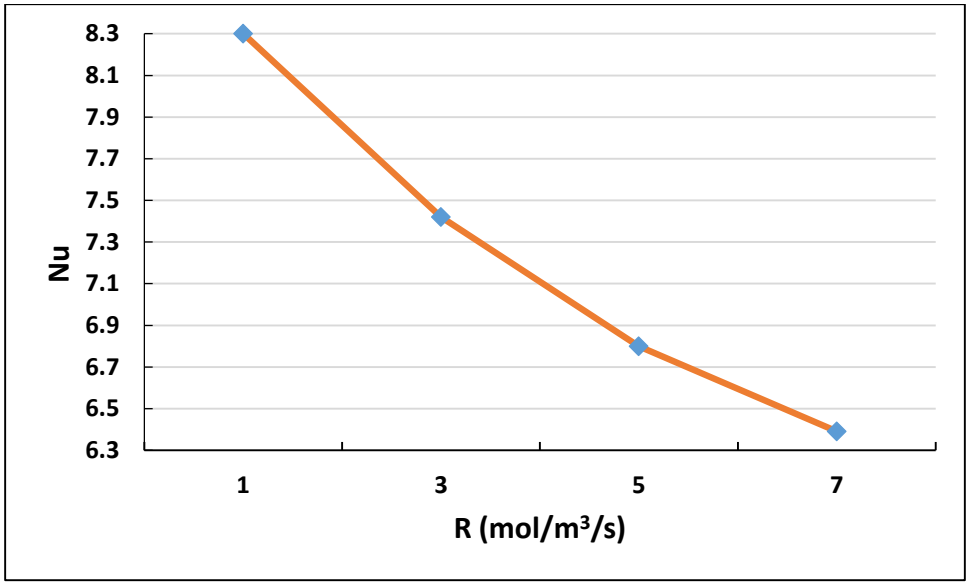


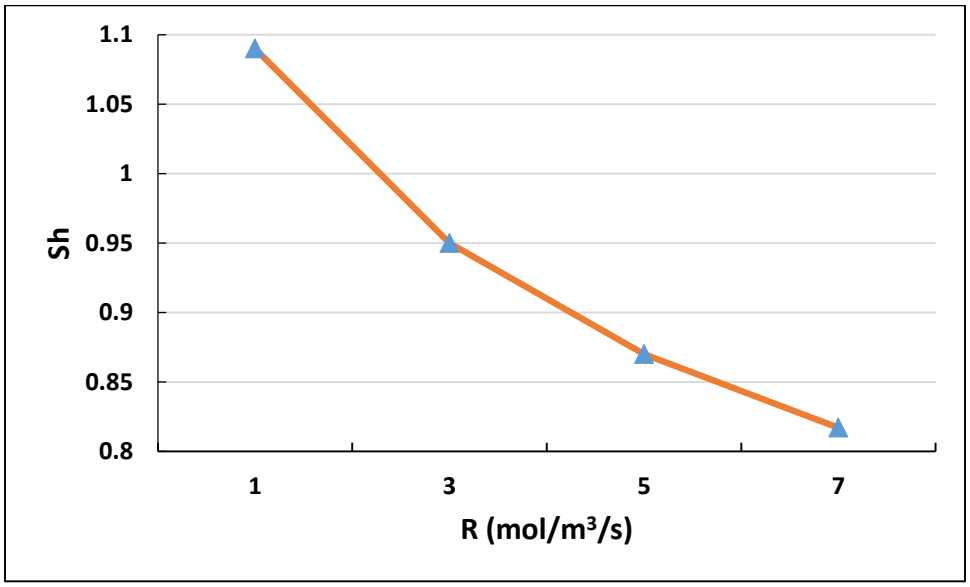
Figure 3.6: Effect of *R* on (a) isotherms, (b) iso-concentration, and (c) streamlines

In Figure 3.7 (i)-(ii) average Nusselt number (*Nu*) at the right hot surface, average Sherwood number (*Sh*) at the inlet in the tubular reactor with the effect of chemical reaction. Increasing *R* decreases the value of *Nu* due to lowering the temperature difference. Heat transfer rate

devalues by 23% with the variation of chemical reaction rate R from 1 to 7 mol/m^3/s. Similarly, reduced mass transfer rate is observed for increasing the rate of chemical reaction through the tubular chemical reactor. The reduction rate of mass transfer (Sh) is 25%. By comparing temperature and mass distributions, one can tell that diffusion to advection (mass) is relatively higher than conduction to convection (heat).



(i)



(ii)

Figure 3.7: Effect of *R* on (i) Nusselt number and (ii) Sherwood number

3.5.3 Effect of solid volume fraction (ϕ)

The performance of water based copper nanoparticles i.e. water-Cu nanofluid in terms of isothermal lines, iso-concentrations, and streamlines are presented in figure 3.8(a) - (c) while H = 10 kJ/mol and R = 1 mol/m^3/s. The values of solid volume fraction of water/alumina nanofluid (ϕ) are considered as 0, 0.5, 1, 2 and 3%. The blue and red colors of each profile indicate the lowest and highest values respectively. From figure 3.10(a), it is noticed that isothermal lines have considerable change due to the variation of solid volume fraction from 0 to 2%. For water-Cu nanofluid with solid concentration ϕ = 0.5% the isothermal lines spreads maximum area of tubular reactor. The temperature lines through the reactor become more heated for growing values of solid volume fraction ϕ from 0.5 to 2%. Cu nanoparticles enhance the thermal conductivity of the water-copper nanofluid. The thermal boundary layer develops for ϕ = 2% at the inlet boundary. But after that there is almost similar pattern in the thermal current activities for ϕ from 2 to 3%.

The profile of iso-concentration has significant change which is shown in figure 3.8(b). Due to increasing concentration the shape of iso-concentration lines become vertical while initially they are bent. This happens because of higher absorptivity of nanoparticles. A little change is observed from this figure for additional mixing (ϕ = 3%) of nanoparticles.

The corresponding velocity field indicates that at ϕ = 0.5% the velocity of nanofluid is high. Thus the streamlines appear the whole tubular reactor. In the velocity vector, initially the flow covers the entire domain of the reactor while it concentrates near the axially symmetric boundary of the reactor due to increase solid volume fraction ϕ from 0.5 to 3% for water-alumina/copper nanofluid. This happens because of escalating solid concentrations of nanofluid flow. Nanofluid having larger density does not move freely.

In figure 3.9 (i)- (ii) average Nusselt number (Nu) at the right hot surface, average Sherwood number (Sh) at the inlet in the tubular reactor with various solid volume fraction are accounted for nanofluid as well as clear water. Rate of heat transfer (Nu) enhances sharply with growing ϕ upto 2% and then remains almost unchanged for advance mixture of solid volume faction for water based nanofluid. Rate of heat transfer enhances by 14% with the

variation of ϕ from 0 to 3% for water-copper nanofluid. Mass transfer rate (*Sh*) at the inlet opening also increases by 20% for increasing values of solid volume fraction from 0 to 3%.

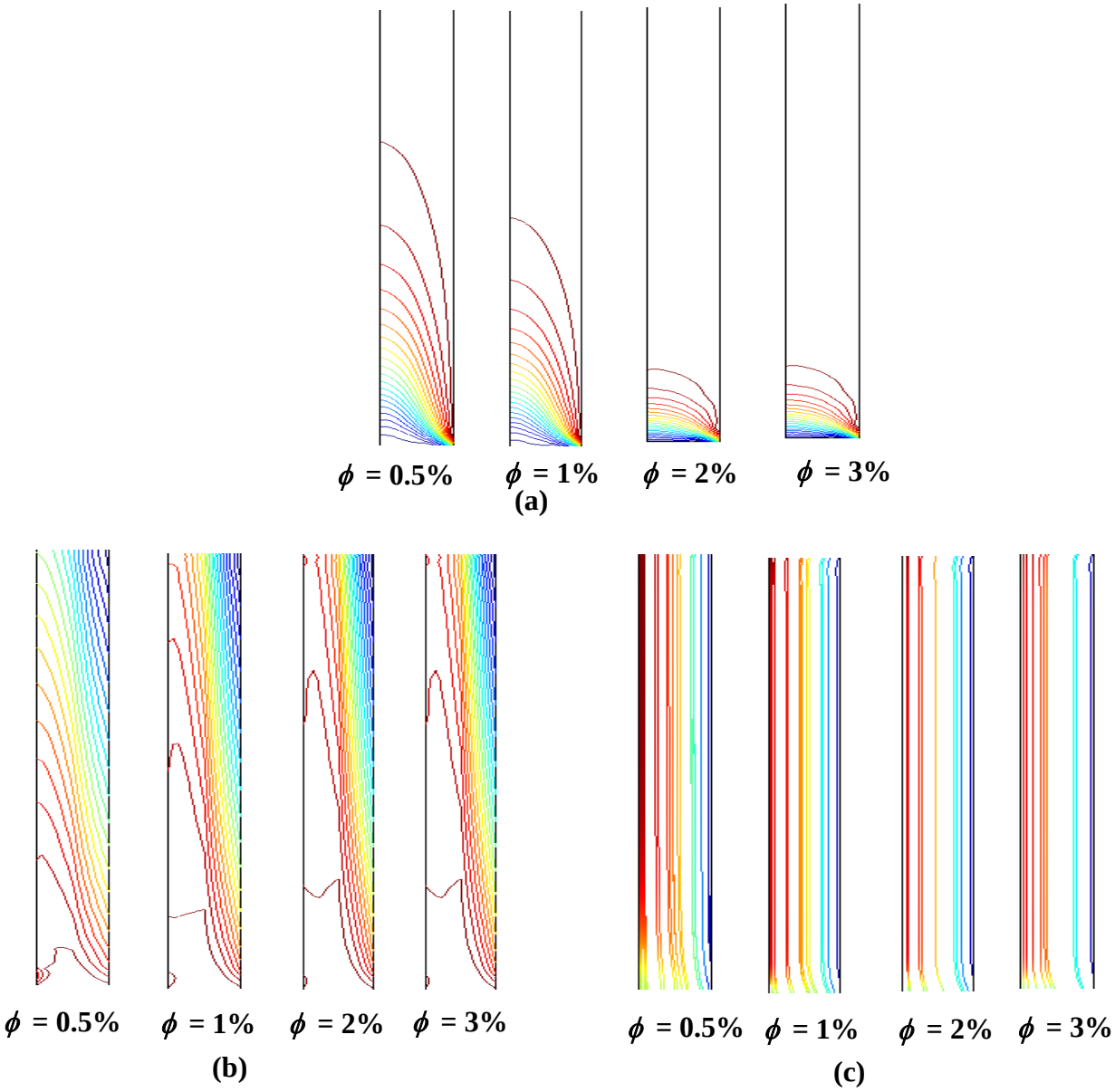
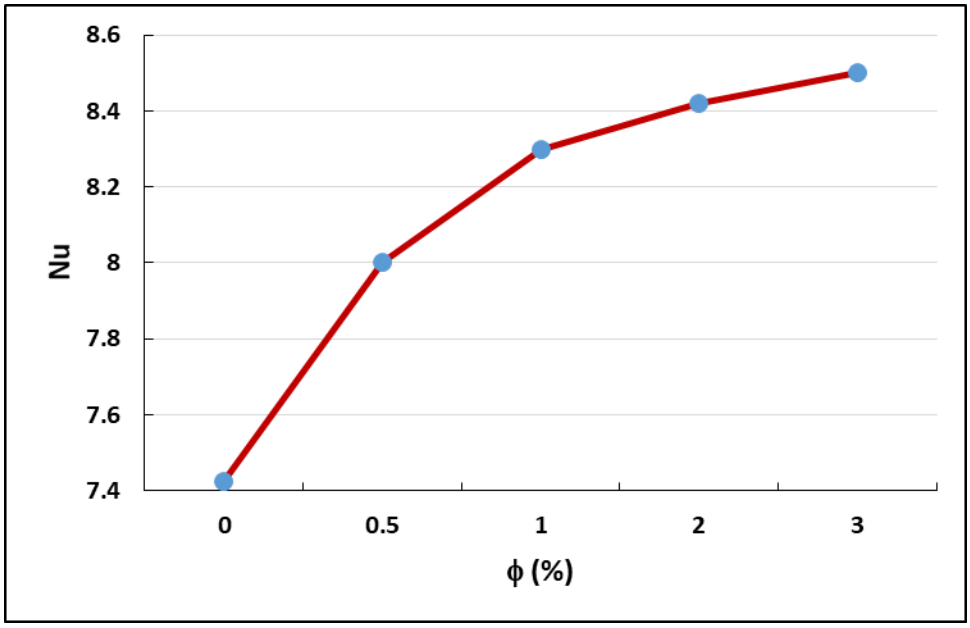
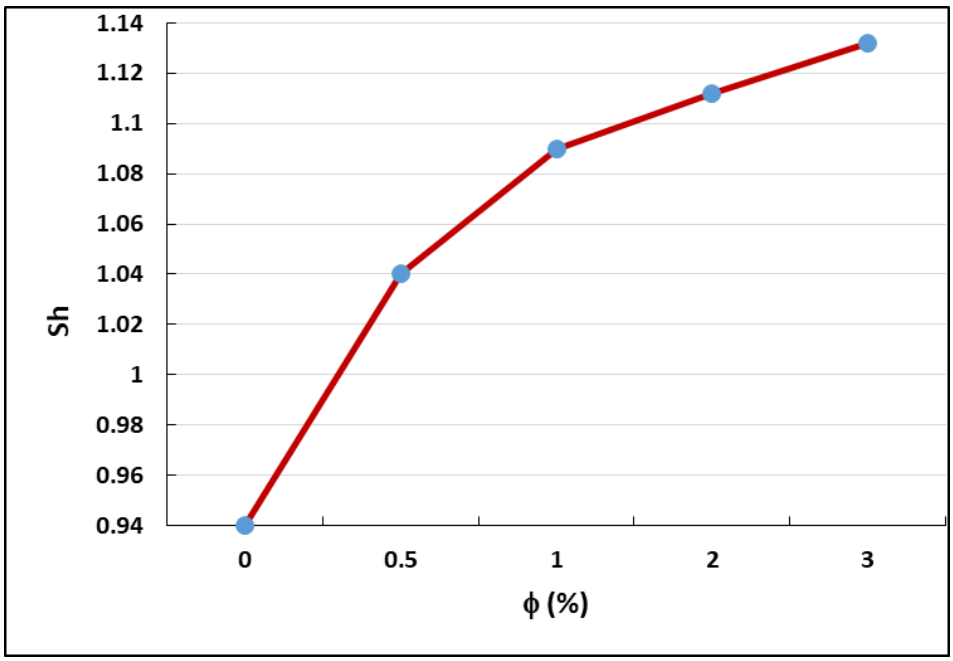


Figure 3.8: Effect of ϕ on (a) isotherms, (b) iso-concentration and (c) streamlines



(i)



(ii)

Figure 3.9: Effect of ϕ on (i) Nusselt number and (ii) Sherwood number

3.5.4 Comparison

The present numerical result has been compared with the result of Kugai [23] for velocity field – radial distance profile of fluid with the graphical representation. Effect of average flow rate on z-velocity has been shown in figure 3.10. Heat and mass transfer on fixed bed tubular reactor was reported by Kugai [23]. Figure 3.10 demonstrates the above stated comparison. As shown in figure 3.10, the numerical solutions of present research and Kugai [23] are in good agreement. The values from the research of Kugai [23] and the present research have been shown also in the Table 3.3. Here percentage of error between these two studies has also been displayed.

Table 3.3 Comparison of velocity magnitude against radius between Kugai [23] and present research

Radius (10^{-3} m)	Velocity field (m/s) obtained from Kugai [23]	Velocity field (m/s) obtained from present result	Error (%)
0	0.61	0.643	5.41
0.5	0.6	0.63	5
1	0.58	0.605	4.31
1.5	0.51	0.535	4.90
1.88	0.4	0.42	5
2	0.36	0.343	4.72
2.125	0.3	0.285	5
2.25	0.2	0.189	5.5
2.375	0.1	0.0952	4.8
2.5	0	0	0

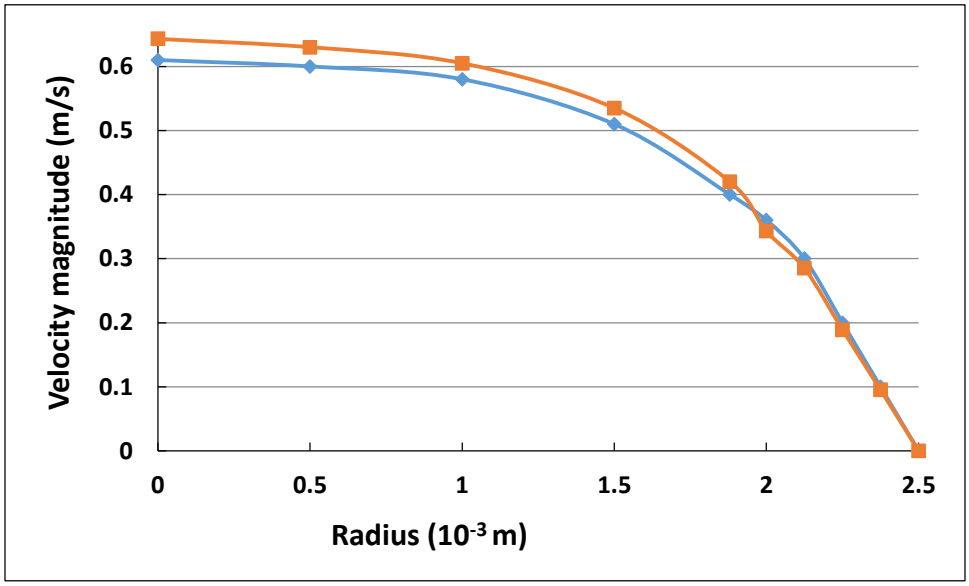


Figure 3.10: Comparison between results of present research (blue color) and Kugai [23] (orange color)

Chapter 4: Conclusions and Recommendations

The problem of finite element modeling of heat and mass transport in a tubular reactor has been studied numerically in this research. The present investigation is done for steady-state, incompressible, laminar and forced convective flow through a tubular chemical reactor. Temperature, concentration and flow fields in terms of isothermal lines, iso-concentration lines and streamlines, respectively have been investigated for various heat of reaction (- 450 - 50 kJ/mol), rate of chemical reaction (1 - 7 mol/m^3/s) and solid concentration (0 - 3%) of water-Cu nanofluid. In addition the heat and mass transfer rates have been calculated and described. The results of the numerical analysis lead to the following conclusions:

4.1 Conclusions

- Perturbation is observed in the conductive and convective heat and mass distribution nearby the right hot wall and inlet opening respectively with the variation of *H*. Decreasing rate of heat and mass transfer are found by 12 and 15%, respectively with rising values of *H*.
- The thermal current activities of the fluid are found to significantly depend upon *R*. The temperature and concentration gradient decrease with rising values of chemical reaction rate. Increasing rate of chemical reaction devalues average *Nu* and *Sh* approximately 23 and 25%, respectively.
- Lower velocity is observed for higher concentrated nanofluid. Increasing ϕ upto 3% causes greater rates of heat and mass transfer by 14 and 20%, respectively compared to base fluid.

4.2 Recommendations

The present research can be extended in future considering the following assumptions:

- ❖ The problems of fluid, heat and mass transfer may be analyzed either theoretically or experimentally.
- ❖ Much theory exists to model the conversion, residence time, reactor size, and other reactor properties based on ideal reactor assumptions, but realistically, those ideal

assumptions are invalid outside of theory. For this reason, it is necessary to study the causes of non-ideal reactors in order to minimize the deviation from the ideal.

- In the light of the above literatures, it is seen that few research have been done with tubular reactor and there is a lot of scope to research with tubular reactor as it has huge applications.

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