

EFFECT OF DOUBLE STRATIFICATION ON BOUNDARY LAYER FLOW AND HEAT OF
NANOFLUID OVER A VERTICAL PLATE IN THE PRESENCE OF CHEMICAL REACTION

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CHAPTER 1

1.1 BACKGROUND

Natural convection is a mechanism, or type of heat transport, in which the fluid motion is not generated by any external source (like a pump, fan, suction device, etc.) but only by density differences in the fluid occurring due to temperature gradients. In natural convection, fluid surrounding a heat source receives heat, becomes less dense and rises. The surrounding, cooler fluid then moves to replace it. This cooler fluid is then being heated and the process continues, forming convection current; this process transfers heat energy from the bottom of the convection cell to top. The driving force for natural convection is buoyancy, a result of differences in fluid density. Natural convection has attracted a great deal of attention from researchers because of its presence both in nature and engineering applications and also their various engineering and industrial applications in heat transfer process. In nature, convection cells formed from air rising above sunlight-warmed land or water are a major feature of all weather systems. Heat transfer by natural convection frequently occurs in many physical problems and engineering application such as geothermal systems, heat exchangers, chemical catalytic reactors, fiber and granular insulation, packed bed, petroleum reservoirs and nuclear waste repositories (Wubshet Ibrahim, 2013 and O.D.Makinde, 2013). Moreover, natural convection of heat and mass transfer occurs in many areas such as in the field of designing chemical processing equipment, distribution of temperature and moisture over agricultural fields and formation and dispersion of fog. In this system heat is transferred from a vertical plate to a fluid moving parallel to it by natural convection. This will occur in any system wherein the density of the moving fluid varies with position. These

phenomena will only be of significance when the moving fluid is minimally affected by forced convection.

Stratification of fluid arises due to temperature variations, concentration differences, or the presence of different fluids. In practical situations where the heat and mass transfer mechanisms run parallel, it is interesting to analyze the effect of double stratification (stratification of medium with respect to thermal and concentration fields) on the convective transport in micro polar fluid. The analysis of free convection in a doubly stratified medium is a fundamentally interesting and important problem because of its broad range of engineering applications. These applications include heat rejection into the environment such as lakes, rivers, and seas; thermal energy storage systems such as solar ponds; and heat transfer from thermal sources such as the condensers of power plants (Minkowycz, 2013). The effect of stratification is an important aspect in heat and mass transfer and has been studied by several researches. In real-world situations where heat and mass transfer run simultaneously, it is significant to investigate the effect of double stratification on the convective transport by using nanofluid. A stratified fluid consisting of fluid parcels of various densities will tend under gravity to arrange itself so that the higher densities are found below lower densities. The vertical layering introduces an obvious gradient of properties in the vertical direction, which affects the velocity. Stratified fluids are universal in nature, present in almost any heterogeneous fluid body such that heterogeneous mixture in industries, salinity stratification in estuaries, density stratification of the atmosphere and many more example (Kaufui Wong, 2010).

Analysis of thermal stratification is very important for solar engineering because higher energy efficiency can be achieved with better stratification and already shown by researchers that the thermal stratification in energy storage may significantly increase system performance. Chen and Eichorn (1998), have been analyzed that natural convective flow over a heated vertical surface in a thermal stratified medium using the local non similarity method for the solution of the governing equations. The study is concerned with a natural convective flow of common fluids by the effects of double stratification on boundary layer flow and heat transfer of nanofluid over a vertical plate in the presence of chemical reaction because nowadays the natural convective flow and heat transfer using nanoparticle suspension in a base fluid has been active research area. The nanofluid is an

advanced type of fluid containing nanometer sized particles (diameter less than 100nm) or fiber suspended in the ordinary fluid. Definitely the nanofluid are beneficial in the sense that the area more stable and have an acceptable viscosity and better wetting, spreading and dispersion properties on a solid surface. Nano fluids are used in different engineering application such as microfluidics, microelectronic, transportation, biomedical, solid state lighting and manufacturing. The research on heat transfer in nanofluid has been receiving increased attention worldwide.

Studies have been shown that a nanoparticle suspension in a base fluid curiously changes the transport property and heat transfer characteristic of a convectional base fluid. A uniform suspension of nanometer size solid particles and fiber in convectional base fluid is called nanofluid. Nano material is a new energy material since its particle size is the same as or smaller than the wavelength of de Broglie wave and coherent wave. Therefore, nanoparticle becomes too strongly absorb and selectively absorbs incident radiation. Based on the radiative motion properties of nanoparticle, the utilization of nanofluid in solar system becomes the new study hotspot. Scientist and engineers today are seeking to utilize solar radiation directly by converting it into useful heat or electricity (Chen and Eichorn, 1998).

Chemical reaction effects on heat and mass transfer are of considerable important in hydrometallurgical industries and chemical technology. In many chemical engineering processes, a chemical reaction occurs between a foreign mass and the fluid. A chemical reaction can be described as either a heterogeneous or homogeneous process, which depend on whether it occurs at an interface or as a single-phase volume reaction. Furthermore, research on combined heat and mass transfer with chemical reaction and thermophoresis effect can help in food processing, cooling towers, chemically reactive vapor deposition boundary layer in optical materials processing, catalytic combustion boundary layers, chemical diffusion in disk electrode modeling and carbon monoxide reactions in metallurgical mass transfer and kinetics. Several investigations have examined the effects of chemical reaction on the flow and heat and mass transfer past a vertical plate (Pooja Sharma, 2011). Although the effect of chemical reaction on heat removal process in nanofluid is important, very little work has been reported in literature.

1.2 PROBLEM STATEMENTS

Nanofluids are engineered by suspending nanoparticles with average size below 100 nm in traditional heat transfer fluids such as water, oil and ethylene glycol. Fluids such as water, oil and ethylene glycol are poor heat transfer fluids since the thermal conductivity of these fluids plays an important role in the heat transfer coefficient between the heat and mass transfer medium and surface. The heat transfer of nanofluid over a vertical plate in the presence of chemical reaction depends on the effects of various governing parameter such as thermal stratification ε_1 , solutal stratification ε_2 , Brownian motion parameter N_b , thermophoresis parameter N_t , buoyancy ratio parameter N_r and chemical reaction γ on velocity $f'(\eta)$, temperature $\theta(\eta)$ and concentration $\phi(\eta)$ profiles. Due to these, following question arise.

1. How does the numerical solution compared to exact solutions?
2. How to obtain a mathematical model relating to the condition involved in the problem?
3. What is the effect of various governing equation such as thermal stratification ε_1 , solutal stratification ε_2 , Brownian motion parameter N_b , thermophoresis parameter N_t , buoyancy ratio parameter N_r and chemical reaction γ on velocity $f'(\eta)$, temperature $\theta(\eta)$ and concentration $\phi(\eta)$ profiles?

1.3 OBJECTIVES OF STUDY

The objectives of this thesis are:-

1. To analyze the effect of various governing parameters such as thermal stratification ε_1 , solutal stratification ε_2 , Brownian motion parameter N_b , thermophoresis parameter N_t , buoyancy ratio parameter N_r and chemical reaction γ on dimensionless velocity $f'(\eta)$, temperature $\theta(\eta)$ and concentration $\phi(\eta)$ profiles.
2. To compare the numerical result on special cases of the problem with previous published result.

1.4 SCOPE OF STUDY

This study is limited to the problem of effect of double stratification on boundary layer flow and heat transfer of nanofluid over a vertical plate in the presence of chemical reaction under some prescribed parameters effects. The prescribed parameters are thermal stratification ε_1 , solutal stratification ε_2 , Brownian motion parameter N_b , thermophoresis parameter N_t , buoyancy ratio parameter N_r and chemical reaction γ on velocity $f'(\eta)$, temperature $\theta(\eta)$ and concentration $\phi(\eta)$ profiles.

The transport equations employed in this analysis which is including the effect of Brownian motion, thermophoresis, thermal stratification and solutal stratification; also the non-linear governing equations and their associated boundary conditions are initially cast into dimensionless forms by similarity variables. The set of equation are highly nonlinear coupled equations and cannot be solved analytically

and numerical solution subject to the boundary condition. Then the set of equations are obtained numerically by using the very robust computer algebra software that is Maple 18. This software uses a fourth –fifth order Runge Kutta Fehlberg method as default to solve boundary value problems numerically using the dsolve command.

1.5 ORGANIZATION OF THE THESIS

Chapter 1 provides some briefing on analysis background, its application in real world, some problem statement, objectives of the analysis, and scope of the study. Chapter 2 presents a literature review on the nanoparticle, nanofluid, thermal stratification, solutal stratification, double stratification, Rayleigh number, Reynolds number, what is chemical reaction either distractive or generative reaction,

Chapter 3 presents the method that will be used along the analysis, how to reduce the governing equation to the dimensionless form, some surface introduction of calculation and some introduction of MAPLE 18 command. It also shows the equations that are used in the shooting technique with MAPLE 18.

Chapter 4 presents the result and discussion on what finding that have been obtained from the simulation, how the prescribe parameters effects on velocity, temperature and concentration profiles. Chapter 5 presents the conclusion on the objectives that has been achieved. Some recommendations for future work are also mentioned in this chapter.

CHAPTER 2

LITERATURE REVIEW

2.0 NANOPARTICLE

Nanoparticles are particles between 1 and 100 nanometers in size. In nanotechnology, a particle is defined as a small object that behaves as a whole unit with respect to its transport and properties. Particles are further classified according to diameter. Ultrafine particles are the same as nanoparticles and between 1 and 100 nanometers in size. Coarse particles cover a range between 2,500 and 10,000 nanometers. Fine particles are sized between 100 and 2,500 nanometers. Nanoparticle research is currently an area of extreme scientific interest due to a wide variety of potential applications in biomedical, optical and electronic fields. Nanoparticles are of great scientific interest as they are, in effect, a bridge between bulk materials and atomic or molecular structures. A bulk material should have constant physical properties regardless of its size, but at the nano-scale size-dependent properties are often observed. Thus, the properties of materials change as their size approaches the nanoscale and as the percentage of atoms at the surface of a material becomes significant. For bulk materials larger than one micrometer (or micron), the percentage of atoms at the surface is insignificant in relation to the number of atoms in the bulk of the material (Kaufi Wong, 2010).

The interesting and sometimes unexpected properties of nanoparticles are therefore largely due to the large surface area of the material, which dominates the contributions made by the small bulk of the material. Suspensions of nanoparticles are possible since the interaction of the particle surface with the solvent is strong enough to overcome density differences, which otherwise usually result in a material either sinking or floating in a liquid. The high surface area to volume ratio of nanoparticles provides a great driving force for diffusion, especially at higher temperatures. Sintering can take place at lower temperatures, over shorter time scales than for larger particles. In theory, this does not affect the density of the final product, though flow difficulties and the tendency of nanoparticles to agglomerate complicates matters. Moreover, nanoparticles have been found to impart some extra properties to various day to day products (Kaufi Wong, 2010).

2.1 NANOFUID

Nanofluid is fluid that contain a nanometer sizes particles which is call nanoparticles where this fluid are engineered colloidal suspension of nanoparticles in a base fluid. Typically nanoparticles are made of from metals, oxides, carbides or carbon nanotubes and common base fluid including water, ethylene glycol and also oil. Nanofluids have novel properties that make them potentially useful in many applications in heat transfer (Minkowyz, 2013) including microelectronics, fuel cells, pharmaceutical processes, engine cooling, vehicle thermal management, domestic refrigerator and heat exchanger. Its show enhanced thermal conductivity and the convective heat transfer coefficient compared to the base fluid (Kakac Sadik and Anchasa Pramuanjaroenkij, 2009).

Nanofluids are dilute liquid suspensions of nanoparticles with at least one of their principal dimensions smaller than 100 nm. From previous investigations, nanofluids have been found to possess enhanced thermophysical properties such as thermal conductivity, thermal diffusivity, viscosity and convective heat transfer coefficients compared to those of base fluids like oil or water (Choi, 2009). Nanofluids are suspensions of nanoparticles in fluids that show significant enhancement of their properties at modest nanoparticle concentrations. Many of

publications on nanofluids is about the understanding of their behaviour so that they can be used where straight heat transfer enhancement is paramount as in many industrial applications, nuclear reactors, transportation, electronics as well as biomedicine and food. Nanofluid as a smart fluid, where heat transfer can be reduced or enhanced at will. Kaufi Wong and Omar De Leon, (2010) focuses on presenting the broad range of current and future applications that involve nanofluids, emphasizing their improved heat transfer properties that are controllable and the specific characteristics that these nanofluids possess that make them suitable for such applications.

In analysis such as computational fluid dynamics (CFD), nanofluids can be assumed to be single phase fluids. However, almost all of new academic papers use two-phase assumption. Classical theory of single phase fluids can be applied, where physical properties of nanofluid are taken as a function of properties of both constituents and their concentrations. An alternative approach simulates nanofluids using a two-component model. Kuznetsov (2013) show that from the current review, it can be seen that nanofluids clearly exhibit enhanced thermal conductivity, which goes up with increasing volumetric fraction of nanoparticles. The current reviews do concentrate on this relatively new class of fluids and not on colloids which are nanofluids because the latter have been used for a long time. Review of experimental studies clearly showed a lack of consistency in the reported results of different research groups regarding thermal properties (Kaufi Wong and Kurma, 2008)

The effects of several important factors such as particle size and shapes, clustering of particles, temperature of the fluid, and dissociation of surfactant on the effective thermal conductivity of nanofluids have not been studied adequately. It is important to do more research so as to ascertain the effects of these factors on the thermal conductivity of wide range of nanofluids. Classical models cannot be used to explain adequately the observed enhanced thermal conductivity of nanofluids. Recently most developed models only include one or two postulated mechanisms of nanofluids heat transfer. For instance, there has not been much fundamental work reported on the determination of the effective thermal diffusivity of nanofluids nor heat transfer coefficients for nanofluids in natural convection. The effects of several important factors such as particle size and shapes, clustering of particles, temperature of the fluid, and dissociation of surfactant on the effective thermal conductivity of nanofluids have not been studied adequately. It is important to do more research so

as to ascertain the effects of these factors on the thermal conductivity of wide range of nanofluids. Classical models cannot be used to explain adequately the observed enhanced thermal conductivity of nanofluids. Recently most developed models only include one or two postulated mechanisms of nanofluids heat transfer. For instance, there has not been much fundamental work reported on the determination of the effective thermal diffusivity of nanofluids nor heat transfer coefficients for nanofluids in natural convection (Choi, 2009)

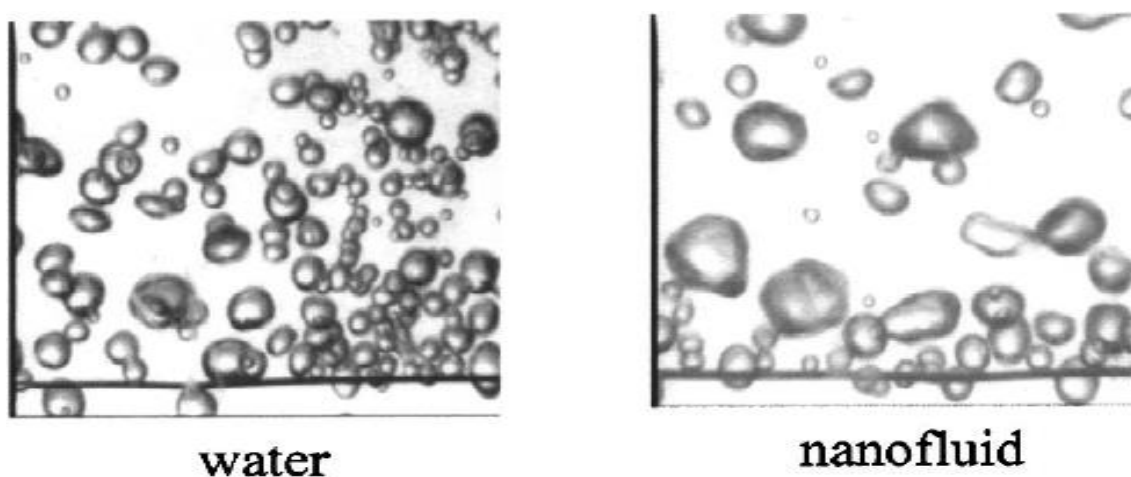


Figure 2. 1: Diagram of water and nanofluid (Choi, 2009)

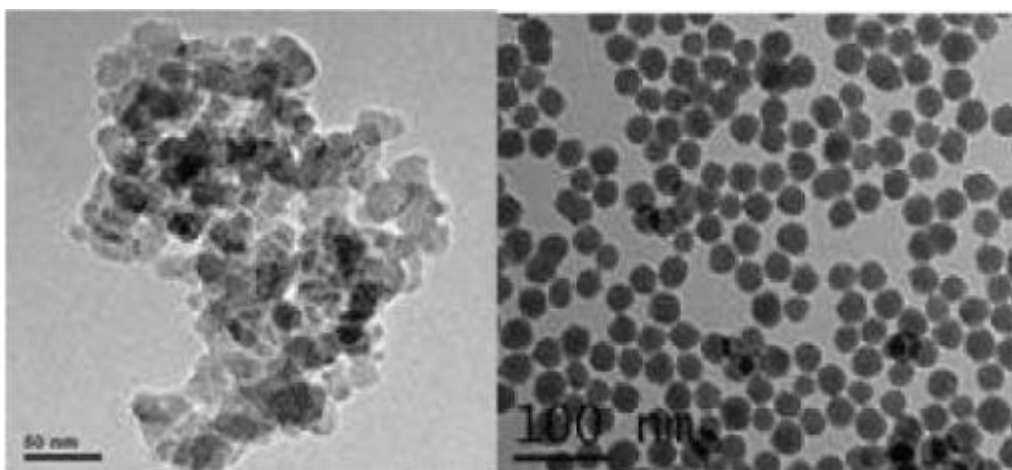


Figure 2.2 : Transmission Electron Microscope (TEM) pictures of nanofluids (Choi, 2009)

Nanofluids are a new class of nanotechnology-based heat transfer fluids engineered by dispersing and stably suspending nanoparticles with typical length on the order of 1–50 nm in traditional heat transfer fluids. For the past decade, pioneering scientists and engineers have made phenomenal discoveries that a very small amount (<1 vol %) of guest nanoparticles can provide dramatic improvements in the thermal properties of the host fluids.

For example, some nanofluids exhibit superior thermal properties such as anomalously high thermal conductivity at low nanoparticle concentrations, strong temperature- and size-dependent thermal conductivity, a nonlinear relationship between thermal conductivity and concentration, and a threefold increase in the critical heat flux at a small particle concentration of the order of 10 ppm. Nanofluids are of great scientific interest because these unprecedented thermal transport phenomena surpass the fundamental limits of conventional macroscopic theories of suspensions. Therefore, numerous mechanisms and models have been proposed to account for these unexpected, intriguing thermal properties of nanofluids.

These discoveries also show that nanofluids technology can provide exciting new opportunities to develop nanotechnology-based coolants for a variety of innovative engineering and medical applications. As a result, the study of nanofluids has emerged as a new field of scientific research and innovative applications. Hence, the subject of nanofluids is of great interest worldwide for basic and applied research. This paper highlights recent advances in this new field of research and shows future directions in nanofluids research through which the vision of nanofluids can be turned into reality (Choi, 2009).

Suspensions of solid submicron and nanometer-sized particles in various fluids (nanofluids) have been considered for applications as advanced heat transfer fluids for almost two decades. However due to the wide variety and the complexity of the nanofluid systems, no agreement has been achieved on the magnitude of potential benefits of using nanofluids for heat transfer applications. Large volume of studies devoted to characterization of individual thermo-physical properties of nanofluids, such as thermal conductivity, viscosity, and agglomeration of nanoparticles has been summarized in a number of review articles (Elena, Wenhua Yu, David and Dileep Singh, 2010).

Evaluation of cooling efficiency, i.e. ability to remove heat from the heat source, includes assessing contributions from thermal conductivity, viscosity, specific heat, and density of the fluid and also depends on the applied flow regime. The studies devoted to evaluation of the heat transfer performance of nanofluids are scarce and inconclusive compared to the studies on the thermo-physical properties of various nanofluids indicating a significant gap between fundamental research and practical applications of nanofluids for thermal management.

2.2 THERMAL STRATIFICATION

Thermal stratification is the scientific term that describes the layering of bodies of water based on their temperature. As water heats and cools, it expands and contracts, changing in density. Still bodies of water including ponds and lakes separate into horizontal layers that have distinctly different temperatures. Each layer of water is stacked above or below the others with the warmest water on top and the coldest on the bottom. Thermal stratification is a natural occurrence, in any static body of water and occurs when the surface layer of water, warmed by the sun, becomes less dense than the water lower it (Wubshet Ibrahim, 2013).

The surface layer remains on top and the lower layer, deprived of surface contact and insulated from the sun, continues to get colder. This increases the difference in density between the two layers and makes it even more difficult for them to mix together. Once strongly established, this stratification persists until falling temperatures in autumn breaks down the density difference between the two layers allowing them to mix together again. In a river, thermal stratification only occurs in the deepest pools if summer flows are insufficient to mix the water in the bottom of the pools. If present it only breaks down when flow increases (Wubshet Ibrahim, 2013).

2.3 DOUBLE STRATIFICATION

Stratification of fluid arises due to temperature variations, concentration differences, or the presence of different fluids. In practical situations where the heat and mass transfer mechanisms run parallel, it is interesting to analyze the effect of double stratification (stratification of medium with respect to thermal and concentration fields) on the convective transport in micropolar fluid. The analysis of free convection in a doubly stratified medium is a fundamentally interesting and important problem because of its broad range of engineering applications. These applications include heat rejection into the environment such as lakes, rivers, and seas; thermal energy storage systems such as solar ponds; and heat transfer from thermal sources such as the condensers of power plants. Although the effect of stratification of the medium on the heat removal process in a fluid is important, very little work has been reported in literature (D.Srinivasacharya, 2010).

2.4 SOLUTAL STRATIFICATION

Influence of stratification is an important aspect in heat and mass transfer analysis. The formation or deposition of the layers is known as the stratification. This phenomenon occurs due to the change in temperature or concentration, or variations in both, or presence of various fluids or different densities. It is quite important and interesting to examine the effects of combined stratifications (thermal and concentration stratifications) in mixed convective flow past a surface when heat and mass transfer analysis is performed simultaneously. Investigation of doubly stratified flows is a subject of special attention nowadays because of its broad range of applications in industrial and engineering processes. Few practical examples of these applications include heat rejection into the environment such as rivers, seas and lakes, thermal energy storage systems like solar ponds, mixture in industrial, food and manufacturing processing (Tariq, 2012). The notion of stratification is essential in lakes and ponds. It is important to control the temperature stratification and

concentration differences of hydrogen and oxygen in such environments such as they may directly affect the growth of all cultured species (Wubshet Ibrahim, 2013). Although the effect of solutal stratification is of the medium on heat removal process in nanofluid is important, very little work has been reported in literature.

2.5 RAYLEIGH NUMBER

In fluid mechanics, the Rayleigh number (Ra) for a fluid is a dimensionless number associated with buoyancy driven flow (also known as free convection or natural convection). When the Rayleigh number is below the critical value for that fluid, heat transfer is primarily in the form of conduction; when it exceeds the critical value, heat transfer is primarily in the form of convection.

The Rayleigh number is named after Lord Rayleigh and is defined as the product of the Grashof number, which describes the relationship between buoyancy and viscosity within a fluid, and the Prandtl number, which describes the relationship between momentum diffusivity and thermal diffusivity. Hence the Rayleigh number itself may also be viewed as the ratio of buoyancy and viscosity forces times the ratio of momentum and thermal diffusivities.

For free convection near a vertical wall, the Rayleigh number is defined as

$$Ra_x = \frac{g\beta}{\nu\alpha} (T_s - T_\infty)x^3 = Pr \quad (2.1)$$

where

x = Characteristic length (in this case, the distance from the leading edge)

R_{ax} = Rayleigh number at position x

Pr = Prandtl number

g = acceleration due to gravity

T_s = Surface temperature (temperature of the wall)

T_∞ = Quiescent temperature (fluid temperature far from the surface of the object)

ν = Kinematic viscosity

α = Thermal diffusivity

β = Thermal expansion coefficient (equals to $1/T$, for ideal gases, where T is absolute temperature)

In the above, the fluid properties Pr , ν , α and β are evaluated at the film temperature, which is defined as

$$T_f = \frac{T_s + T_\infty}{2} \quad (2.2)$$

For most engineering purposes, the Rayleigh number is large, somewhere around 106 to 108.

For a uniform wall heating flux, the modified Rayleigh number is defined as

$$Ra_x = \frac{g\beta q_0''}{\nu\alpha k} x^4 \quad (2.3)$$

where

q_0'' = the uniform surface heat flux (W/m²)

k = the thermal conductivity (W/m•K)

2.6 REYNOLDS NUMBER

In fluid mechanics, the Reynolds number (Re) is a dimensionless quantity that is used to help predict similar flow patterns in different fluid flow situations. The concept was introduced by George Gabriel Stokes in 1851 but the Reynolds number is named after Osborne Reynolds (1842–1912), who popularized its use in 1883.

The Reynolds number is defined as the ratio of inertial forces to viscous forces and consequently quantifies the relative importance of these two types of forces for given flow conditions.[5] Reynolds numbers frequently arise when performing scaling of fluid dynamics problems, and as such can be used to determine dynamic similitude between two different cases of fluid flow. They are also used to characterize different flow regimes within a similar fluid, such as laminar or turbulent flow:

- laminar flow occurs at low Reynolds numbers, where viscous forces are dominant, and is characterized by smooth, constant fluid motion;
- turbulent flow occurs at high Reynolds numbers and is dominated by inertial forces, which tend to produce chaotic eddies, vortices and other flow instabilities.

In practice, matching the Reynolds number is not on its own sufficient to guarantee similitude. Fluid flow is generally chaotic and very small changes to shape and surface roughness can result in very different flows. Nevertheless, Reynolds numbers are a very important guide and are widely used.

The Reynolds number can be defined for several different situations where a fluid is in relative motion to a surface. These definitions generally include the fluid properties of density and viscosity, plus a velocity and a characteristic length or characteristic dimension. This dimension is a matter of convention – for example radius and diameter are equally valid to describe spheres or circles, but one is chosen by convention. For flow in a pipe or a sphere moving in a fluid the internal diameter is generally used today. Other shapes such as rectangular pipes or non-spherical objects have an equivalent diameter defined. For fluids of variable density such as compressible gases or fluids of variable viscosity such as non-Newtonian fluids,

special rules apply. The velocity may also be a matter of convention in some circumstances, notably stirred vessels. The Reynolds number is defined below for each case.

$$Re = \frac{\text{inertial forces}}{\text{viscous forces}} = \frac{\rho v L}{\mu} = \frac{v L}{\nu} \quad (2.4)$$

where:

v is the mean velocity of the object relative to the fluid (SI units: m/s)

L is a characteristic linear dimension, (travelled length of the fluid; hydraulic diameter when dealing with river systems) (m)

μ is the dynamic viscosity of the fluid (Pa·s or N·s/m² or kg/(m·s))

ν is the kinematic viscosity ($\nu = \mu/\rho$) (m²/s)

ρ is the density of the fluid (kg/m³).

Note that multiplying the Reynolds number by $\frac{\rho L v}{\rho L v}$ yields $\frac{\rho v^2 L^2}{\mu v L}$, which is the ratio of the inertial forces to the viscous forces. It could also be considered the ratio of the total momentum transfer to the molecular momentum transfer.

2.7 CHEMICAL REACTION

A chemical reaction is a process that leads to the transformation of one set of chemical substances to another. Classically, chemical reactions encompass changes that only involve the positions of electrons in the forming and breaking of chemical bonds between atoms, with no change to the nuclei (no change to the elements present), and can often be described by a chemical equation. Nuclear chemistry is a sub-discipline of chemistry that involves the chemical reactions of unstable and radioactive elements where both electronic and nuclear changes may occur (Srinivasacharya, 2014).

The substance (or substances) initially involved in a chemical reaction are called reactants or reagents. Chemical reactions are usually characterized by a chemical change, and they yield one or more products, which usually have properties different from the reactants. Reactions often consist of a sequence of individual sub-steps, the so-called elementary reactions, and the information on the precise course of action is part of the reaction mechanism. Chemical reactions are described with chemical equations, which graphically present the starting materials, end products, and sometimes intermediate products and reaction conditions (Srinivasacharya, 2014).

Chemical reactions happen at a characteristic reaction rate at a given temperature and chemical concentration, and rapid reactions are often described as spontaneous, requiring no input of extra energy other than thermal energy. Non-spontaneous reactions run so slowly that they are considered to require the input of some type of additional energy (such as extra heat, light or electricity) in order to proceed to completion (chemical equilibrium) at human time scales (Beltrame P, 2010).

Different chemical reactions are used in combinations during chemical synthesis in order to obtain a desired product. In biochemistry, a similar series of chemical reactions form metabolic pathways. These reactions are often catalyzed by protein enzymes. These enzymes increase the rates of biochemical reactions, so that metabolic syntheses and decompositions impossible under ordinary conditions

may be performed at the temperatures and concentrations present within a cell (Beltrame P, 2010).

The general concept of a chemical reaction has been extended to reactions between entities smaller than atoms, including nuclear reactions, radioactive decays, and reactions between elementary particles as described by quantum field theory. Homogeneous reactions are chemical reactions in which the reactants are in the same phase, while heterogeneous reactions have reactants in two or more phases. Reactions that take place on the surface of a catalyst of a different phase are also heterogeneous (Srinivasacharya, 2012).

A reaction between two gases or two miscible liquids is homogeneous. A reaction between a gas and a liquid, a gas and a solid or a liquid and a solid is heterogeneous. A mixture can be determined to be homogeneous when everything is settled and equal, and the liquid, gas, object is one colour or the same form. Various models have been proposed to model the concentrations in different phases. The phenomena to be considered are mass rates and reaction (Beltrame P, 2010).

2.8 REACTION RATE

The rate of a reaction is the speed at which a chemical reaction happens. If a reaction has a low rate, that means the molecules combine at a slower speed than a reaction with a high rate. Some reactions take hundreds, maybe even thousands, of years while others can happen in less than one second. If you want to think of a very slow reaction, think about how long it takes plants and ancient fish to become fossils (carbonization). The rate of reaction also depends on the type of molecules that are combining. If there are low concentrations of an essential element or compound, the reaction will be slower. The reactions happen over and over, but not always at the same speed. A few things affect the overall speed of the reaction and the number of collisions that can occur (Beltrame P, 2010).

Temperature: When you raise the temperature of a system, the molecules bounce around a lot more. They have more energy. When they bounce around more, they are more likely to collide. That fact means they are also more likely to combine. When you lower the temperature, the molecules are slower and collide less. That

temperature drop lowers the rate of the reaction. To the chemistry lab sometimes you will mix solutions in ice so that the temperature of the system stays cold and the rate of reaction is slower (Beltrame P, 2010).

Concentration: If there is more of a substance in a system, there is a greater chance that molecules will collide and speed up the rate of the reaction. If there is less of something, there will be fewer collisions and the reaction will probably happen at a slower speed. Sometimes, when you are in a chemistry lab, you will add one solution to another. When you want the rate of reaction to be slower, you will add only a few drops at a time instead of the entire beaker (Beltrame P, 2010).

Pressure: Pressure affects the rate of reaction, especially when you look at gases. When you increase the pressure, the molecules have less space in which they can move. That greater density of molecules increases the number of collisions. When you decrease the pressure, molecules don't hit each other as often and the rate of reaction decreases. Pressure is also related to concentration and volume. By decreasing the volume available to the molecules of gas, you are increasing the concentration of molecules in a specific space. You should also remember that changing the pressure of a system only works well for gases. Generally, reaction rates for solids and liquids remain unaffected by increases in pressure (Beltrame P, 2010).

A chemical system, unless it is already in equilibrium, tends to evolve towards this state and does so at a specific velocity, which is called the reaction rate. Reaching equilibrium may take a fraction of a second or several years, but in all cases it takes time. How long it takes depends on the reaction and on the circumstances under which it takes place. The branch of chemistry that studies these facts is called chemical kinetics (Beltrame P, 2010).

The reaction rate (r) is usually defined as the number of moles of a given reactant that react per unit time and per unit volume:

$$r = \frac{\text{moles reacted}}{\text{times} \times \text{volume}} \quad (2.5)$$

Since some reactions occur on surface it is possible, in these cases to define the reaction rate as the number of moles reacting per unit time and per unit surface.

However, the material that forms the reaction surface will be probably enclosed within a volume, so even in these cases the reaction rate r defined above is reasonable reference (Beltrame P, 2010).

The variables that affect the reaction rate are essentially the concentration of the reactant(s) and the temperature. In this case of gas-phase reactions, the former variable may usefully be expressed as partial pressure of the reactant(s).

The mathematical expression indicating how r depends on the variables is termed the rate equation. It contains at least one kinetic coefficient (k), but may also contain other coefficients. The simplest example is a rate equation of the form:

$$r = kC_A \tag{2.6}$$

where C_A is the molar concentration of a reactant A.

CHAPTER 3

METHODOLOGY

3.1 OVERVIEW

In this chapter, the method that has been applied will be described in more details. The transport equations employed in this analysis which is including the effect of Brownian motion, thermophoresis, thermal stratification and solutal stratification; also the non-linear governing equations and their associated boundary conditions are initially cast into dimensionless forms by similarity variables. The set of equation are highly nonlinear coupled equations and cannot be solved analytically and numerical solution subject to the boundary condition. Then the set of equations are obtained numerically using the very robust computer algebra software that is Maple 18. This software uses a fourth – fifth order Runge Kutta Fehlberg method as default to solve boundary value problems numerically using the dsolve command.

The transformed system of coupled nonlinear ordinary differential equations and the boundary conditions are depending on some governing parameters. The numerical result obtained are presented in the form of dimensionless velocity, temperature, nanoparticle volume fraction and concentration profiles and been shown graphically.

3.2 MATHEMATICAL FORMULATION

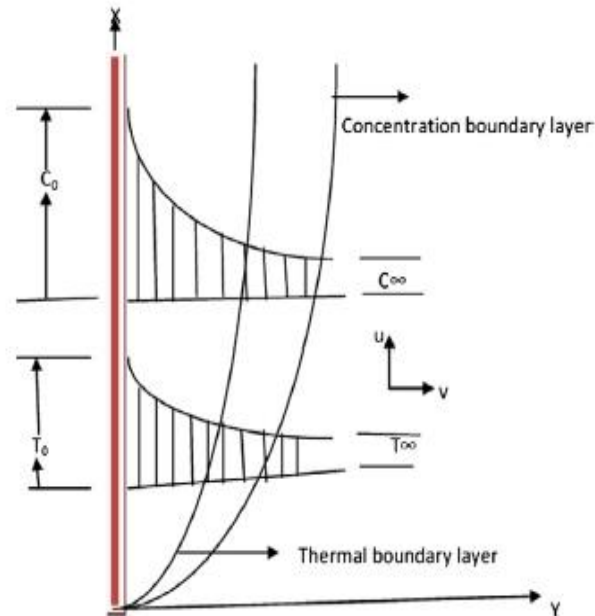


Figure 3.1: Flow configuration and coordinate system

Consider the steady state free convective along a vertical plate embedded in a stable doubly stratified nanofluid as shown in Figure 3.1. We choose the coordinate system such that the x -axis is along the vertical plate and y -axis is normal to the plate. The temperature and the concentration of the ambient medium are assumed to be linearly stratified in the form of $T_{\infty}(x) = T_{\infty,0} + Ax$ and $C_{\infty}(x) = C_{\infty,0} + Bx$ respectively where A and B are constants and varied to alter the intensity of stratification in the medium: $T_{\infty,0}$ and $C_{\infty,0}$ are ambient temperature and ambient concentration respectively. The body surface is kept at a constant temperature T_w and concentration C_w .

Using the standard boundary layer approximation, the governing equations for the continuity, momentum and energy in boundary layer flow can be written as

$$\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} = 0 \quad (3.01)$$

$$u \frac{\partial u}{\partial x} + v \frac{\partial u}{\partial y} = v \frac{\partial^2 u}{\partial y^2} + (1 + \phi_{\infty,0}) \rho_{f\infty,0} \beta g (T - T_{\infty,0}) - (\rho_p - \rho_{f\infty,0}) g (\phi - \phi_{\infty,0}) \quad (3.02)$$

$$\frac{\partial T}{\partial y} + v \frac{\partial T}{\partial y} = \alpha \frac{\partial^2 T}{\partial y^2} + \tau \left\{ D_B \frac{\partial \phi}{\partial y} \frac{\partial T}{\partial y} + \frac{D_T}{T_{\infty}} \left(\frac{\partial T}{\partial y} \right)^2 \right\} \quad (3.03)$$

$$u \frac{\partial \phi}{\partial x} + v \frac{\partial \phi}{\partial y} = D_B \frac{\partial^2 \phi}{\partial y^2} + \left(\frac{D_T}{T_{\infty}} \right) \left(\frac{\partial^2 T}{\partial y^2} \right) - K_1 \phi \quad (3.04)$$

with boundary conditions as

$$f(0) = 0, f' = 0, \quad \theta(0) = 1 - \frac{\varepsilon_1}{4}, \quad h(0) = 1 - \frac{\varepsilon_2}{4} \quad \text{at } \eta = 0 \quad (3.05)$$

$$f'(\infty) = 0, \quad \theta(\infty) = 0, \quad h(\infty) = 0, \quad \text{as } \eta \rightarrow \infty \quad (3.06)$$

Where u, v is the velocity of component along x and y direction. $\phi_{\infty,0}$ is the nanoparticle volume fraction at a large value of y , ϕ is the nanoparticle volume fraction at the surface. $\rho_{f\infty,0}$ is the density of the fluid, β is volume expansion coefficient, T is the temperature of the fluid inside the boundary layer while $T_{\infty,0}$ is the ambient temperature. ρ_p is the effective heat capacity of a nanoparticle, $\rho_{f\infty,0}$ is heat capacity of the fluid, α is thermal diffusivity, $\tau = \frac{(\rho c)_p}{(\rho c)_f}$, D_B is Brownian diffusion coefficient and D_T is thermophoresis diffusion coefficient. ε_1 is thermal