ANALYSIS OF BOUNDARY LAYER FLOW OF NANOFUID WITH THE CHARACTERISTICS OF HEAT AND MASS TRANSFER

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ANALYSIS OF BOUNDARY LAYER FLOW OF NANOFUID WITH THE
CHARACTERISTICS OF HEAT AND MASS TRANSFER

By
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211269573

Thesis submitted in fulfilment of the requirements for the degree of Master
of Technology
In the Department of Mechanical Engineering
Cape Peninsula University of Technology
Bellville Campus
South Africa

Supervisor: Senior Professor O. D. Makinde

November 2011
DECLARATION

I, Olanrewaju Anuoluwapo Mary, declare that the content of this thesis represent my own work and has not been submitted previously for academic examination towards any qualification. Furthermore, it represents my own opinions and not necessarily those of the Cape Peninsula University of Technology.

Signed: ..................................................  Date: 13/02/2012

Analysis of Boundary Layer Flow of Nanofluid with the Characteristics of Heat and Mass Transfer

Olanrewaju A.M
ABSTRACT

Nanofluid, which was first discovered by the Argonne laboratory, is a nanotechnology-based heat transfer fluid. This fluid consists of particles which are suspended inside conventional heat transfer liquid or base fluid. The purpose of this suspension is for enhancing thermal conductivity and convective heat transfer performance of this base fluid. The name nanofluid came about as a result of the nanometer-sized particles of typical length scales 1-100nm which are stably suspended inside of the base fluids. These nanoparticles are of both physical and chemical classes and are also produced by either the physical process or the chemical process.

Nanofluid has been discovered to be the best option towards accomplishing the enhancement of heat transfer through fluids in different unlimited conditions as well as reduction in the thermal resistance by heat transfer liquids. Various manufacturing industries and engineering processes such as transportation, electronics, food, medical, textile, oil and gas, chemical, drinks e.t.c, now aim at the use of this heat transfer enhancement fluid. Advantages such organisations can obtain from this fluid includes, reduced capital cost, reduction in size of heat transfer system and improvement of energy efficiencies.

This research has been able to solve numerically, using Maple 12 which uses a fourth-fifth order Runge-Kutta-Fehlberg algorithm alongside shooting method, a set of nonlinear coupled differential equations together with their boundary conditions, thereby modelling the heat and mass transfer characteristics of the boundary layer flow of the nanofluids. Important properties of these nanofluids which were considered are viscosity, thermal conductivity, density, specific heat and heat transfer coefficients and microstructures (particle shape, analysis of boundary layer flow of nanofluid with the characteristics of heat and mass transfer Olanrewaju A.M
volume concentration, particle size, distribution of particle, component properties and matrix-particle interface).

Basic fluid dynamics equations such as the continuity equation, linear momentum equation, energy equation and chemical species concentration equations have also been employed.

Furthermore, the effects of various parameters controlling the flow system such as Prandtl number (Pr), Lewis number (Le), Biot number (Bi), Thermophoresis (Nt), Brownian motion (Nb) Suction/Injection β, the local skin friction coefficient, the reduced Nusselt number (Nur) and reduced Sherwood number (Shr) are worked out as well. In order to significantly provide a better understanding on the dynamics of nanofluids and to augment its usefulness in all fields applicable. This research has established mathematically the usefulness of nanofluids over conventional fluids.
DEDICATION

I dedicate this thesis to God Almighty and to all who indeed are less privileged all over the world.

Analysis of Boundary Layer Flow of Nanofluid with the Characteristics of Heat and Mass Transfer
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ACKNOWLEDGEMENTS

My utmost appreciation goes to the Almighty God, my maker and the master planner of my life. Thank you Jesus.

How can I ever appreciate Professor O.D Makinde, Senior Professor and Director of the centre for post graduate studies, Cape Peninsula University of Technology, You have been my driving force, my motivation and inspiration. The drillings, fatherly roles and your advice have gone farther than you may imagine. I will forever acknowledge you. Thank you Sir.

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Oyindamola and Samuel, my lovely kids, thank you for your endurances and sacrifices. I love you both.

My loved ones, home and abroad, I appreciate every bit of the encouragements you all gave me.

I thank National Research Foundation (NRF) for their financial support during the course of this research work.
## NOMENCLATURE

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<thead>
<tr>
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<td>$C$</td>
<td>nanoparticle volume fraction</td>
</tr>
<tr>
<td>$C_f$</td>
<td>skin-friction coefficient</td>
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<tr>
<td>$C_w$</td>
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<td>$C_\infty$</td>
<td>nanoparticle volume fraction at free stream</td>
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<td>$D_B$</td>
<td>Brownian diffusion</td>
</tr>
<tr>
<td>$D_T$</td>
<td>thermophoretic diffusion coefficient</td>
</tr>
<tr>
<td>$k$</td>
<td>thermal conductivity</td>
</tr>
<tr>
<td>$Le$</td>
<td>Lewis number</td>
</tr>
<tr>
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<td>Brownian motion parameter</td>
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<td>$q_{w}$</td>
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</tr>
<tr>
<td>$q_{m}$</td>
<td>surface heat flux</td>
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<tr>
<td>$t$</td>
<td>time</td>
</tr>
<tr>
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<td>$T_f$</td>
<td>temperature of the fluid</td>
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<td>$Nur$</td>
<td>reduced Nusselt number</td>
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<table>
<thead>
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<td>$h$</td>
<td>convective heat transfer coefficient</td>
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<td>$u, v$</td>
<td>velocity component along $x$ and $y$ directions respectively</td>
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<td>$\infty$</td>
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<td>thermal diffusivity of the base fluid</td>
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<td>concentration at the sheet surface</td>
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<td>temperature at the sheet surface</td>
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<td>density of the base fluid</td>
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<td>$\rho_p$</td>
<td>density of the particle</td>
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<td>$(\rho c)_\rho$</td>
<td>heat capacity of the base fluid</td>
</tr>
<tr>
<td>$(\rho c)_\rho$</td>
<td>heat capacity of the nanoparticle material</td>
</tr>
<tr>
<td>$\tau$</td>
<td>rate of heat capacity</td>
</tr>
<tr>
<td>$\nu$</td>
<td>kinematic viscosity of the base fluid</td>
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<td>$\psi$</td>
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<td>$\beta$</td>
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<td>$\vec{q}$</td>
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CHAPTER

1. Introduction

Nanofluids are nanotechnology-based heat transfer fluids, which consists of particles suspended inside of liquids (typically conventional heat transfer liquids). They have been shown to enhance thermal conductivity and convective heat transfer performance of the base liquids. The name was discovered by Argonne National Laboratory to describe this fluid because of nanometer-sized particles (of typical length scales 1 to 100nm) that are stably suspended inside of the base liquid. Moreover, many industrial processes require the transfer of heat through a flowing fluid either in laminar or turbulent regime, flowing or stagnant boiling fluids in a large range of temperature and pressure. Reduction in thermal resistance of heat transfer liquids will serve as a benefit to many of these applications in terms of reduced capital cost, reduction of size of heat transfer system and improvement of energy efficiencies. These can be achieved in nanofluids and various industries and manufacturing organizations such as transportation, electronics, medical and food stand to benefit a lot in these improved heat transfer fluids.

Nanoparticles are regarded as a class of materials with unique properties both chemical and physical and they are fabricated materials at nanometer scale. The production of these particles can then be classified into two, namely the physical process and chemical processes. Examples of nanoparticles which have been commonly used are oxide ceramics (Al_2O_3, Analysis of Boundary Layer Flow of Nanofluid with the Characteristics of Heat and Mass Transfer Olanrewaju A.M)
CuO), Nitride ceramics (AlN, SiN), carbide ceramics (SiC, TiC), metals (Ag, Au, Cu, Fe), semiconductors (TiO₂), single-, double- or multi-walled carbon nanotubes (SWCNT, DWCNT, MWCNT), and the composite materials such as nanoparticle core-polymer shell composites. However, new materials and structures are attractive for use in nanofluids where the particle-liquid interface is doped with various molecules. Nanoparticles are mostly produced in the form of powder and are dispersed in aqueous or organic host liquids to form nanofluids for specific applications. Physical processes include mechanical grinding method and the inert-gas-condensation technique (developed by Granqvist and Buhrman [55]). The chemical processes include chemical precipitation, chemical vapour deposition, micro-emulsions, spray pyrolysis, and thermal spraying. A sonochemical method has been developed to make suspensions of iron nanoparticles stabilized by oleic acid (Kenneth, et al [76]).

Figure 1.1: (a) is the image of amorphous carbonic nanofluids and (b) is the image of alumina nanofluids

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Figure 1.2: Semi micrograph of ZnO nanoparticles

Meanwhile, boundary layer refers to that region of a fluid which forms in the vicinity of a surface bounding a fluid. It occurs when fluid flows in pipes and channels, wind moves around structures or buildings, over the wings of aeroplanes, the surface of moving vehicles, e.t.c. The movement of fluid molecules over surfaces creates regions near the surfaces which greatly affects the dynamics of both the fluid and the object. The flow in the region surrounding a body can be divided into the boundary layer and anywhere outside of the boundary. Outside of the boundary layer, the viscosity on the body is negligible, and the flow may be treated as inviscid. Therefore, only flow inside the boundary layer is important for determining frictional resistance, Fox et al [47].

The most important development in the study of fluid mechanics occurred during the 20th century when Prandtl [136] introduced his concepts of boundary layer. Prandtl’s theory states that due to the no-slip condition, the velocity of fluid molecules at the surface of a stationery...
body is zero, but the velocity given by the inviscid flow theory is reached within a thin layer closed to the surface called the ‘boundary layer’. David et al [34] and Tulapurkara [164] indicated that Prandtl’s 1904 paper on the subject formed the basis for future works on skin friction, heat and mass transfer and separation in the boundary layer. The details of flow within the boundary layer are very important for many problems in aerodynamics. Prandtl’s concepts led to improve designs of objects and bodies moving in fluids such as aeroplanes, ships, rockets, cars, pipelines, etc. The present study investigates mathematically the effects of various controlling parameters on the boundary layer flow of nanofluids with heat and mass transfer characteristics.

![Figure 1.3: Sketch of boundary layer](image)

Analysis of Boundary Layer Flow of Nanofluid with the Characteristics of Heat and Mass Transfer

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1.1 Applications of nanofluids.

Various applications of nanofluids can be found in transportation, microelectronics, defence, nuclear, space, and biomedical as highlighted below:

1.1.1 Transportation

Conventional or base fluids such as, water, ethylene glycol, water mixture and engine oil in the order of their performance in heat transfer from the highest to the lowest are yet poor heat transfer fluids. When nanoparticles are stably dispersed into standard engine coolant it tends to improve automotive and heavy-duty engine cooling rates. This improvement serves a lot of benefits, examples, reduction in coolant system size and weight and this benefit all parts of the vehicle and its performance also fuel conservation. Furthermore, improved cooling rates
for truck engines and any other automotives can remove more heat from higher horsepower engines with the same size of coolant system. As earlier stated, pure ethylene glycol is a poor heat transfer fluid compared to a mixture of ethylene glycol and water in the same proportion. Nevertheless, the addition of nanoparticles improves the enhancement. The higher boiling point characteristic of nanofluid coolant can be used to increase the normal coolant operating temperature, and then reject more heat through the existing coolant system. The more heat is being rejected, the more variety of design enhancements is being allowed in engines and with ones of higher horsepower.

Tzeng et al. [165] performed an experiment on the platform of transmission of a four-wheel drive; this transmission had an advanced rotary blade coupling, where high local temperatures occurred at high rotating speeds using engine transmission oil in which he suspended CuO and Al₂O₃ nanoparticles. The temperature distribution on the exterior of the rotary-blade-coupling transmission was measured at four engine operating speeds (400, 800, 1200, and 1600rpm), and the optimum composition of nanofluids with regard to heat transfer performance was investigated. From the results it was deduced that CuO nanofluids produced the lowest transmission hence, the application of nanofluids in transmission is of great advantage in terms of thermal conductivity.

Zhang and Que [203] point out that surface-modified nanoparticles are detected to be effective in enhancing tribological properties such as reducing wear and reducing the friction between moving mechanical components when these particles are stably dispersed in mineral oils. This accounts for the application of nanofluid in automotive lubrication.
1.1.2 Electronics Cooling

The increase in microprocessors and integrated circuits have been in the recent years a dramatic one. It was predicted by International Technology Roadmap for Semiconductors that by 2018, high performance integrated circuits will contain more than 9.8 billion transistors on a chips of 90-nm node size. Also processors for high-performance computers and servers have been predicted to dissipate higher power in the range of 100-300W/cm$^2$ in future. Single-phase fluids are candidate replacements for air-cooling techniques for removing heat as liquid cooling technology investigations for heat transfer increases.

Tsai et al [162], experimented a circular heat pipe designed as heat spreader to be used in a CPU in a notebook or a desktop PC using water- based nanofluid and the experiment shows a significant decrease in thermal resistance of the heat pipe compared with deionised water. The results showed the effects of nanoparticles size on the thermal resistance of a vertical meshed heat pipe. Ma et al.[106] also investigated the effect of nanofluids on the heat transport capability of an oscillating heat pipe experimentally, it has been proven that, a nanofluid containing 1vol.% nanoparticles with input power of 80W, reduced the temperature difference between the evaporator and the condenser is reduced from 40.9°C to 24.3°C. Hence this result and others encourages more research on the application of nanofluids.

1.1.3 Defence

A high-heat-flux cooling of about tens of MW/m$^2$ is required in quite a number of military devices, as a result of this, the use of convention fluids as cooling fluids is challenging. For examples, the cooling of power electronics and energy directed- weapons which involve high
heat fluxes more than 500-1000 W/cm². Nanofluids have a potential of providing adequate cooling for them and the associated power electronics as well as providing the required cooling in other military equipments and machines such as military vehicles, submarines, and high-power laser diodes. Other areas of nanofluid research for defence applications includes multifunctional nanofluids with added thermal energy storage or energy harvesting feat, transformer cooling in the navy as well as in power generation industry having the objective of reducing the size and weight of transformers. The projective demand for greater production of electricity can also lead to the replacement or improvement of transformer on a large scale and at a high cost. Nanofluid as it has been demonstrated, could significantly improve the heat transfer properties of transformer oils.

1.1.4 Space

You [198] and Vassalo et al. [170] reported order of magnitude increasing in the critical heat flux in a pool boiling, with comparing nanofluids to base fluids. The tendency of raising chip power in electronic components or simplifying cooling requirements for space applications is being presented. High critical heat fluxes which allows for boiling to higher qualities with increased heat removal and wider safety margin from film boiling makes nanofluids attractive in general electronic cooling as well as space applications with very high power density.

1.1.5 Nuclear Systems Cooling

An interdisciplinary centre for nanofluid technology for the nuclear energy industry has been established by the Massachusetts Institute of Technology. In this institute, evaluations of the
impact and use of nanofluids on safety, neutronic and economic functions of nuclear systems are being examined. The use of nanofluids in the place of water in a Pressurized Water Reactor (PWR), makes the fuel rod becomes coated with nanoparticles such as alumina and prevents the formation of a layer vapour around the rod and subsequently increasing the critical heat flux significantly. Nanofluids are also useful in the geothermal power and other energy sources.

1.1.6 Biomedicine

In order to circumvent some side effects of local methods of cancer treatment, iron-based nanoparticle could be used as delivery vehicles for drugs or radiation without affecting the surrounding tissues, hence reducing organ damage. Nanoparticles could be guided in the bloodstream to a tumour using magnets external to the body. More so, nanofluids could be used to provide effective cooling around the surgical region hence improving safe surgery which thereby enhances patient’s chance of survival.

Jordan, et al. [71] however reported that nanofluid could also be used to produce a higher temperature around the tumours to kill cancerous cells without affecting nearby healthy cells.

1.2 Properties of nanofluids

The properties of nanofluids such as viscosity, thermal conductivity, density and specific heat and heat transfer coefficient are effectively measured. And this is done when details of their microstructures (such as particle shape, component volume concentration, particle size, distribution of particle, component properties, and matrix-particle interfacial effects) are fully
known. The term “Matrix” is used to define nanofluids for theoretical modelling purpose. Prandtl number (named after the German physics Ludwig Prandtl) is a dimensionless quantity of momentum diffusivity (Kinematic viscosity) to thermal diffusivity and is hence defined as,

\[
Pr = \frac{\nu}{\alpha} = \frac{C_p \mu}{k} \frac{Viscosity \text{ diffusion rate}}{thermal \text{ diffusion rate}},
\]

Where \( \nu = \text{Kinematic viscosity}, \frac{\mu}{\rho} (\text{S.I. units} : m^2/s) \),

\( \alpha = \text{Thermal diffusivity}, \frac{k}{\rho C_p} (\text{S.I. units} : m^2/s) \),

\( \mu = \text{Dynamic viscosity}, (\text{S.I. units} : w/(m.k)) \),

\( C_p = \text{Specific heat}, (\text{S.I. units} : J/(kg.k)) \),

\( \rho = \text{Density}, (\text{S.I. units} : kg/m^3) \).

1.3 Literature Review

Heat transfer enhancement brought about by the excellent potentials of nanofluids has propelled both industry and universities to launch research and development efforts in nanotechnology after the pioneering demonstrations and experiments by Argonne Laboratory. Nanofluids exhibit increases in thermal performances as compared to the conventional heat transfer fluids. Choi et al. [25] in their study reveal that the addition of less than 1% volume of nanoparticles to conventional heat transfer liquids increased the thermal conductivity of the fluids approximately twice. Another important property of nanofluids is a stronger...
temperature-dependent thermal conductivity than in the ordinary base fluid (Das et al. [29]). Many researchers have determined the thermal conductivity enhancement of different nanoparticles in a variety of liquids with volume concentrations to be in the range of 0.5-4%. At these low particle volume concentrations, typical enhancement has been in the 25% range over the base fluid parameter in forced-convection cooling applications, including engines and thermal systems. More importantly, experiments have shown that nanoparticles significantly enhance the heat transfer coefficient of flowing liquids as reported by (Faulkner, et al. [46]).

Table 1.1: Models showing the effective heat transfer coefficient of nanofluids:

<table>
<thead>
<tr>
<th>Model</th>
<th>Equation</th>
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<tbody>
<tr>
<td>Pak and Cho [130] (for Al₂O₃-in-water and TiO₂-in-water nanofluids, turbulent flow)</td>
<td>( Nu = 0.021Re^{0.8}Pr^{0.5} )</td>
</tr>
<tr>
<td>Das, et al. [30] (Al₂O₃-in-water nanofluids, pool boiling)</td>
<td>( Nu = cRe_b^{m}Pr^{0.4} ), where c and m are particle volume concentration dependent parameters.</td>
</tr>
<tr>
<td>Xuan and Li [188] (for CuO-in-water nanofluids, turbulent flow)</td>
<td>( Nu = 0.0059(1.0 + 7.6286\nu_0^{0.6886}Pe_\nu^{0.001})Re^{0.9238}Pr^{0.4} )</td>
</tr>
<tr>
<td>Yang, et al. [193], (for graphite-in-transmission fluid and graphite-in-synthetic oil mixture nanofluids, laminar flow)</td>
<td>( Nu = cRe^{m}Pr(D/L)^{1/2}(\mu_b/\mu_w)^{0.14} ) where c and m are nanofluid and temperature dependent empirical parameters.</td>
</tr>
<tr>
<td>Buongiorno [20] (turbulent)</td>
<td>( Nu = \frac{(f/8)(Re-1000)Pr}{1+\delta_v^+ (f/8)^{1/2} (Pr_c^{2/3} L)} ) where the dimensionless thickness of the laminar sublayer ( \delta_v^+ ) is an empirical.</td>
</tr>
</tbody>
</table>

Furthermore, the increase of viscosity of nanofluids as compared to that of conventional fluids has been investigated by many researchers. Although experimental data for effective viscosity of nanofluids are limited to certain nanofluids, such as;
- \(\text{Al}_2\text{O}_3\) in water (Park and Cho [129]; Das, et al. [30], Putra, et al. [141]; Li, et al. [95]; Heris, et al. [63]),
- \(\text{CuO}\) in water (Heris, et al [63]; Kulkarni, et al. [87]),
- \(\text{TiO}_2\) in water (Park and Cho [129]),
- MWCNT in water (Ding, et al. [38]),
- \(\text{Al}_2\text{O}_3\) in octane (Liu, et al. [96]).

This experimental data show the trend that the effective viscosities of nanofluids are higher than the theoretical predictions and the ranges of the parameters (the particle volume concentration, temperature, etc.) are limited. Researchers then proposed equations applied to specific applications e.g., \(\text{Al}_2\text{O}_3\) in water (Ma'ga, et al. [108]), \(\text{Al}_2\text{O}_3\) in ethylene glycol (Ma'ga, et al. [108]), and \(\text{TiO}_2\) in water (Tseng and Lin [163]). Kulkarni et al [87] proposed an equation for \(\text{CuO}\) in water taking temperature into consideration. Wang and Wei [174] developed an exact equivalence between the dual phase-lagging heat conduction in nanofluids. Abu-Nada [1] investigated numerically the heat transfer over a backward step (BFS) using nanofluids. Oztop and Abu-Nada [129] studied theoretically the problem of steady boundary layer flow of a nanofluid past a moving semi-infinite flat plate in a uniform free stream. Duangthongsuk and Wongwises [33] investigated the effects of the thermophysical properties on the predicted values of convectional heat transfer coefficient in \(\text{TiO}_2\)-water nanofluid flowing through a horizontal double-tube counter flow heat exchangers under turbulent flow conditions. Oztop and Abu-Nada [129] performed a numerical study to investigate the effect of using different nanofluids on natural convection flow field and temperature distributions in partially heated square enclosure from the left vertical wall. Nield and Kuznetsov [128] examined the influence of nanoparticles on natural convection.
boundary layer flow in a porous medium past a vertical plate. Dongsheng Wen et al. [40] conducted a critical review of the state-of-the-art nanofluids research for heat transfer applications and conclude that current understanding on nanofluids is still quite limited. Syakila and Loan [157] studied the steady mixed convection boundary layer flow past a vertical flat plate embedded in a porous medium filled with nanofluids using different nanoparticles such as Al₂O₃, Cu, TiO₂. Hamad et al. [59] studied the hydromagnetic free convection boundary layer flow past a semi-infinite flat plate embedded in water filled with a nanofluid. Kuznetsov and Nield [90] examined the natural convective boundary layer flow of nanofluids over a vertical plate. The model used for the nanofluids incorporates the effect of Brownian motion and thermophoresis. Cyril Okhio et al. [28] investigated the flow characteristics and heat transfer coefficient of nanofluids under laminar forced convection over a flat plate. Khan and Pop [79] studied the problem of boundary layer flow of nanofluids over a stretching flat surface numerically.

1.4 Statement of the problem

In many industrial and engineering processes, where improved heat transfer in terms of capital and cost of production, the quality and quantity, nanofluid is a better option for the accomplishment of the enhancement in heat transfer performance in various different and unlimited conditions. An illustration is the reservation of energy in a heating, ventilating and air conditioning systems which is obtained without necessarily increasing the pumping power in buildings as a result of nanofluid application while providing environmental benefits. Furthermore, nanofluid coolant also have application potentials in major industrial systems such as material, chemical, food, textile, paper printing, drink, oil and gas. In order to
improve the effectiveness of nanofluid, it is extremely important to understand the inherent complex dynamics of the flow systems. In this research project a mathematical model for boundary layer flow of nanofluids with heat and mass characteristics will be investigated.

1.5 Research aims and Objective

The main aim of this research is to provide a mathematical model for boundary layer flow of nanofluids with heat and mass transfer characteristics. In order to achieve this goal, our objectives include;

- to derive a mathematical model for boundary layer flow of nanofluids
- to analyse the model using appropriate numerical technique
- to investigate the effects of various embedded parameters controlling the flow system on skin friction together with heat and mass transfer rate
- to establish mathematically the usefulness of nanofluids over conventional fluids in industrial and engineering processes.

1.6 Methodology

Modelling real systems like boundary layer flow of nanofluids do involve solving a system of nonlinear differential equations. The model will be derived from the basic equations governing the boundary layer flow of nanofluids which include: the continuity, momentum, energy and concentration balance equations. The problem will be solved numerically using shooting method coupled with fourth order Runge-Kutta integration scheme. Relevant
software like Maple will be utilised to develop a numerical code that will be implemented on a computer.

### 1.6.1 Shooting Methods

Shooting method is a numerical technique of analysing some common two-point boundary value problems. This iterative algorithm technique is usually used to guess the initial conditions for a related boundary value problem (BVP), hence transforming a BVP to an initial value problem (IVP). Fourth order Runge-Kutta Iteration scheme is then employed to solve the resulting IVP. Shooting methods reforms the two-point value problems as a nonlinear parameter estimation problem which is majorly the need for this technique. Solution for the reformulated problem is expected to satisfy the approximated boundary conditions at the other end point with the initial conditions chosen. This process is repeated until the limit of the iteration is attained or the expected accuracy is achieved. A mathematical illustration is expressed below;

Consider the two-point BVP for a system of $n$ first-order ODEs.

$$
\frac{dy}{dt} = f(t, y(t)),
$$

$$
y_i(a) = \alpha_i, \quad i = 1, 2, \ldots, m_1.
$$

$$
y_{m_1+j}(b) = \beta_j, \quad j = 1, 2, \ldots, m_2. \quad 1.1
$$

The vector $y$ contains the $n$ unknown functions of the independent variable $t$. The initial $m_1 (0 < m_1 < n)$ components of $y$ have first order boundary conditions as the unknown functions are ordered. The remaining $m_2 := n - m_1$ components of the solution have first
order boundary conditions specified at a second point, \( t = b \) (note; (1.1) is an initial value problem if \( m_2 = 0 \).

The shooting method recognises the vector of parameters \( s \in \mathbb{R}^{m_2} \) so that the solution, denoted by \( y(t; s) \), to the initial value problem

\[
\begin{align*}
\frac{dy}{dt} &= f(t, y(t; s)), \\
y_i(a; s) &= \alpha_i, & i = 1, 2, \ldots, m_1. \\
y_{m_i+1}(a; s) &= s_j, & j = 1, 2, \ldots, m_2.
\end{align*}
\]

agrees with the solution to (1.1). Note that (1.2) is the same as (1.1) with the boundary conditions at present \( t = b \) replaced with unknown initial conditions at \( t = a \) to determine the correct initial values, consider the “objective function” \( F \) with components

\[
F_j(s) := y_{m_i+1}(b; s) - \beta_j, & j = 1, 2, \ldots, m_2.
\]

This implies that (1.1) can be solved if and only if there exists \( s \in \mathbb{R}^{m_2} \) such that \( F(s) = 0 \). Obtaining the desired result of this process depends majorly on the iterative procedure used to construct a sequence of parameter vectors that converges to a zero of \( F \). Any numerical root-finding algorithm could be used for this step but the mostly used method is one step of the Newton-Raphson method. This means that given an initial guess \( s^0 \in \mathbb{R}^{m_2} \), define the sequence of initial conditions \( \{s^k\} \) by

\[
s^{k+1} := s^k - \left( \nabla F(s^k) \right)^{-1} F(s^k)
\]

for all \( k \geq 0 \). In order to implement this, it is important to note that the vector \( F(s^k) \) is directly obtained from the solution of (1.2), but the Jacobian matrix \( \nabla F(s^k) \) require the
values of \( \frac{\partial x_{i+1}(y, s^k)}{\partial s_j} \) for all \( i, j = 1,2,...,m_2 \). These values can be obtained by solving the \( n \) IVPs in (1.2) alongside the \( nm_2 \) sensitivity equations:

\[
\frac{d}{dt} \left( \frac{\partial y_i}{\partial s_j} \right) = \frac{\partial f}{\partial y_i} \frac{\partial y_i}{\partial s_j}, \quad i = 1,2,...,n, \quad j = 1,2,...,m_2.
\]

With corresponding initial conditions

\[
\frac{\partial y_i}{\partial s_j} = 0, \quad \text{for all} \quad i = 1,...,m_1, \quad j = 1,2,...,m_2.
\]

\[
\frac{\partial y_{m+1}}{\partial s_j} = 0, \quad \text{for all} \quad i, j = 1,...,m_2.
\]

1.7 Significance

The output of this study will provide a better understanding on the dynamics of nanofluids and thereby augment its usefulness in various industrial and engineering processes like chemical and manufacturing industries, defence, biomedical, transportation etc.
2 Fluid Dynamics Equations

2.1 Continuity Equation

In continuous fluid motion, if we consider a surface $S$ fixed in a space containing a volume $V$, it is clear that the increase in the mass of the fluid that flows in the system is the same as the mass of the fluid that flows out. The mass of the fluid within the system is

$$\int \rho \, dv.$$  \hspace{1cm} (2.1)

The rate of increase of the mass within the surface is given as

$$\frac{\partial}{\partial t} \int \rho \, dv = \int \frac{\partial \rho}{\partial t} \, dv.$$ \hspace{1cm} (2.2)

Consider the following diagram and the fluid within the surface,

![Flow continuity diagram](image)

**Figure 2.1:** Flow continuity diagram.
Since volume $V$ does not vary with time, the rate of flow through $S$ is,

$$
\int_S \left( \bar{q} \cdot \vec{n} \right) \rho ds = \int_V \nabla \cdot (\rho \bar{q}) dv ,
$$

(2.3)

$$
\int_V \frac{\partial \rho}{\partial t} dv = - \int \nabla \cdot (\rho \bar{q}) dv ,
$$

(2.4)

$$
\int_V \frac{\partial \rho}{\partial t} dv + \int_V \nabla \cdot (\rho \bar{q}) dv = 0 ,
$$

(2.5)

$$
\int_V \left( \frac{\partial \rho}{\partial t} + \text{div} (\rho \bar{q}) \right) dv = 0 .
$$

(2.6)

This is valid for any arbitrary volume $V$, the integral must identically vanish. Thus, we obtain,

$$
\frac{\partial \rho}{\partial t} + \text{div} (\rho \bar{q}) = 0 .
$$

(2.7)

Equation (2.7) is called continuity equation for any fluid and it can be written as,

$$
\frac{\partial \rho}{\partial t} + \rho \text{div} \bar{q} + (\bar{q} \cdot \nabla) \rho = 0 .
$$

(2.8)

But

$$
\frac{D}{Dt} + \rho \text{div} \bar{q} = 0 .
$$

(2.9)

Where

$$
\frac{D}{Dt} = \frac{\partial}{\partial t} + \bar{q} \cdot \nabla ,
$$

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is the material derivative, which represents differentiation following fluid motion. For incompressible motion we have

\[
div \vec{q} = 0. \quad (2.10)
\]

If \( \vec{q} = (u, v, w) \), then

\[
\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} + \frac{\partial w}{\partial z} = 0. \quad (2.11)
\]

If the fluid is incompressible, but two dimensional we have,

\[
\frac{\partial u}{\partial x} + \frac{\partial v}{\partial x} = 0, \quad (2.12)
\]

then one can (or may) introduce the function \( \psi \) given by,

\[
u = \frac{\partial \psi}{\partial y}, v = -\frac{\partial \psi}{\partial x}. \quad (2.13)
\]

This equation satisfies the continuity equation:

\[
u_x + u_y = (\psi_y)_x + (-\psi_x)_y = \psi_{yx} - \psi_{xy} = 0,
\]

\[-\frac{\partial^2 \psi}{\partial x \partial y} + \frac{\partial^2 \psi}{\partial x \partial y} = 0. \quad (2.14)
\]

Now if the flow is irrotational then,
This implies that there exists a scalar function $\phi$ such that,

$$q = -\nabla \phi.$$  \hspace{1cm} (2.16)

In two dimensions, we have,

$$u = \frac{\partial \phi}{\partial x}, v = -\frac{\partial \phi}{\partial y}.$$  \hspace{1cm} (2.17)

From equation (2.12), we obtain,

$$\frac{\partial^2 \phi}{\partial x^2} + \frac{\partial^2 \phi}{\partial y^2} = 0.$$  \hspace{1cm} (2.18)

### 2.2 Momentum Equation

Consider a small parallel pipe of volume $dV = dx_1 \times dx_2 \times dx_3$, isolated instantaneous from the fluid with centre $(x_1, x_2, x_3)$ we shall denote by $\sigma_{ij}$ the stress acting in the $X_i$ direction on the force whose normal lies in the $X_j$ direction. The stress component $\sigma_{11}, \sigma_{12}, \sigma_{13}, \ldots$ from a second order stress tensor $\sigma_{ij}$

i.e

$$\sigma_{ij} = \begin{bmatrix} \sigma_{11} & \sigma_{12} & \sigma_{13} \\ \sigma_{21} & \sigma_{22} & \sigma_{23} \\ \sigma_{31} & \sigma_{32} & \sigma_{33} \end{bmatrix}.$$  \hspace{1cm} (2.19)
This is called the stress matrix. The components $\sigma_{ij}$ are the normal stress while the components $\sigma_{ij}^{(i\neq j)}$ are shearing stresses. The shear tensor and the corresponding matrix are symmetric i.e., $\sigma_{ij} = \sigma_{ji}$. In relation to a surface at the right angles to the axis $x_j$, the stress per unit area at $(x_1 + x_2 + x_3)$ and $\sigma_{11}, \sigma_{12}, \sigma_{13}$. The corresponding stresses as the centre of the forces are given as:

\[
\begin{align*}
\sigma_{11} &= \frac{1}{2} \frac{\partial \sigma_{11}}{\partial x_1} dx_1, \\
\sigma_{12} &= \frac{1}{2} \frac{\partial \sigma_{12}}{\partial x_1} dx_1, \\
\sigma_{13} &= \frac{1}{2} \frac{\partial \sigma_{13}}{\partial x_1} dx_1,
\end{align*}
\]

(2.20)

using Taylor expansion in the form

\[
\sigma_{11}(x_1, x_2, x_3) = \sigma_{11}(x_1, x_2, x_3) + \frac{1}{2} \frac{\partial \sigma_{11}}{\partial x_1} dx_1.
\]

(2.21)

At the centre of the opposite force, the corresponding stresses are

\[
\begin{align*}
\sigma_{11} &= \frac{1}{2} \frac{\partial \sigma_{11}}{\partial x_1} dx_1, \\
\sigma_{12} &= \frac{1}{2} \frac{\partial \sigma_{12}}{\partial x_1} dx_1, \\
\sigma_{13} &= \frac{1}{2} \frac{\partial \sigma_{13}}{\partial x_1} dx_1
\end{align*}
\]

(2.22)

acting on the fluid in parallel compound. The stresses on a pair of opposite force may be compounded into

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\[
\frac{\partial \sigma_{11}}{\partial x} \, dx_1, dx_2, dx_3,
\]
\[
\frac{\partial \sigma_{12}}{\partial x} \, dx_1, dx_2, dx_3,
\]
\[
\frac{\partial \sigma_{13}}{\partial x} \, dx_1, dx_2, dx_3,
\]
\[
\frac{\partial \sigma_{21}}{\partial x_2} + \frac{\partial \sigma_{22}}{\partial x_2} + \frac{\partial \sigma_{23}}{\partial x_2} \right) dx_1, dx_2, dx_3. \tag{2.23}
\]

acting at \((x_1 + x_2 + x_3)\) parallel to \((0 \, x_1 + 0 \, x_2 + 0 \, x_3)\). The stress on the other two pairs opposite forces may be compounded into similar forces at \((x_1 + x_2 + x_3)\). The resultant force in \(x_i\) the direction becomes

\[
\left( \frac{\partial \sigma_{11}}{\partial x_1} + \frac{\partial \sigma_{12}}{\partial x_2} + \frac{\partial \sigma_{13}}{\partial x_3} \right) dx_1, dx_2, dx_3. \tag{2.24}
\]

If \(X, Y, Z\) are the forces per unit area due to variation of stress along \(0 \, x_1 + 0 \, x_2 + 0 \, x_3\), then

\[
X = \frac{\partial \sigma_{11}}{\partial x_1} + \frac{\partial \sigma_{12}}{\partial x_2} + \frac{\partial \sigma_{13}}{\partial x_3} = \frac{\partial \sigma_{\alpha 1}}{\partial x_\alpha}, \alpha = 1, 2, 3.
\]

\[
Y = \frac{\partial \sigma_{21}}{\partial x_1} + \frac{\partial \sigma_{22}}{\partial x_2} + \frac{\partial \sigma_{23}}{\partial x_3} = \frac{\partial \sigma_{\alpha 2}}{\partial x_\alpha}, \alpha = 1, 2, 3.
\]

\[
Z = \frac{\partial \sigma_{31}}{\partial x_1} + \frac{\partial \sigma_{32}}{\partial x_2} + \frac{\partial \sigma_{33}}{\partial x_3} = \frac{\partial \sigma_{\alpha 3}}{\partial x_\alpha}. \tag{2.25}
\]

Generally, we denote the body of forces by \(F = (F_1, F_2, F_3) = F_i, i = 1, 2, 3\) then the equation of motion is given by:

\[
\rho \frac{\partial u_i}{\partial t} = \frac{\partial \sigma_{ij}}{\partial x_i} + F_i. \tag{2.26}
\]
In tensor notation we have $\mathbf{q} = (U_1, U_2, U_3) = U_i, i = 1,2,3$ i.e., the velocity vector. It is convenient to regard the stress $\sigma_{ij}$ as the sum of inviscid part $-p\sigma_{ij}\delta_{ij}$ and a viscous part $\sigma_{ij}$ where $p$ is the average of the three normal stresses for any orthogonal set of axes

$$p = \frac{\sigma_{ij}}{3}\delta_{ij} = \frac{1}{3}(\sigma_{11} + \sigma_{22} + \sigma_{33}),$$

(2.27)

where $\delta_{ij}$ is the substitution tensor.

Now separate the second tensor $\frac{\partial U_i}{\partial x_j}$ as follows:

$$\frac{\partial U_i}{\partial x_j} = \frac{1}{2}\left(\frac{\partial U_i}{\partial x_j} + \frac{\partial U_i}{\partial x_j}\right) + \frac{1}{2}\left(\frac{\partial U_i}{\partial x_j} + \frac{\partial U_i}{\partial x_i}\right),$$

$$= \frac{1}{2}e_{ij} + \frac{1}{2}\gamma_{ij}.$$  

(2.28)

$e_{ij}$ is the symmetric tensor while $\gamma_{ij}$ is the anti-symmetric rotational tensor defining the velocity of the motion. In uniform media viscous stress are induced only by deformation and not by rotation $e_{ij}$ is called rate of strain tensor. It represents the rate of change in the size and shape of a fluid element. The momentum equation now becomes

$$\rho \frac{d\mathbf{q}}{dt} + (\mathbf{q} \cdot \nabla)\mathbf{q} = -\nabla P + \nabla \cdot \mathbf{\sigma} + \rho F.$$  

(2.29)
2.3  Energy Equation

In order to derive energy equation, we need to consider the zeroth and the first law of thermodynamics.

2.3.1  The Zeroth Law of Thermodynamics

There exists the temperature \( T \), such that when two systems that are in contact are in thermal equilibrium, then \( T \) is the same in both systems. \( T \) is called the absolute temperature.

2.3.2  The First Law of Thermodynamics

This law expresses the principle of conservation of energy such that energy can not be created or destroyed. The law states that there exists a variable of state \( E \) such that if a system is transformed from one state of equilibrium to another by the process in which an amount of work \( E \) is done on the system by its surroundings and an amount of heat \( Q \) is added to the system from the surrounding. The difference between the initial and final values of energy of the systems \( E_i \) and \( E_f \) is given by

\[
E_f - E_i = Q + W ,
\]  

(2.30)

in differential form we have

\[
dE = dQ + dW ,
\]  

(2.31)

or
\[
\frac{dE}{dt} = \frac{dQ}{dt} + \frac{dW}{dt} .
\]

(2.32)

In order to determine the work, we consider the contribution from the component \( \sigma_{ij} \) of stress. The work in unit time is given by

\[
\frac{\partial (W \sigma_{xx})}{\partial t} = dydz \left\{ -U \sigma_{xx} + \left( U + \frac{\partial U}{\partial x} dx \right) \left( \sigma_{xx} + \frac{\partial \sigma_{xx}}{\partial x} dx \right) \right\} = \Delta V \frac{\partial (U \sigma_{xx})}{\partial x} ,
\]

(2.33)

where,

\[ \nabla V = dx dy dz . \]

The total work done by the stress per unit mass on deforming elements of fluid \( \Delta V \) is given by

\[
\frac{1}{\rho} \frac{\partial \left( \sigma_{ij} U_{j} \right)}{\partial x_{i}} = \frac{1}{2} \left( \frac{\partial \sigma_{ij}}{\partial x_{i}} + \sigma_{ij} \frac{\partial U_{j}}{\partial x_{i}} \right) ,
\]

(2.34)

where \( \sigma_{ij} \) is the stress acting in the \( x_{i} \) on the force normal lies in the \( x_{j} \) direction.

For the equation of fluid motion, we have

\[
\rho \frac{\partial U_{i}}{\partial t} = \frac{\partial \left( \sigma_{ij} \right)}{\partial x_{i}}
\]

(2.35)

and

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which is clearly the change in kinematic energy of fluid element following motion. The remaining term in equation (2.35) represents the rate of dissipation of energy per unit mass.

Substituting $\sigma_{ij} = p\delta_{ij} + \mu e_{ij},$

$$\frac{\partial W}{\partial t} = \frac{1}{2} \frac{\partial (U_j U_j)}{\partial t} - \frac{p}{\rho} \sigma_{ij} \frac{\partial U_j}{\partial x_i} + \nu \frac{\partial U_i}{\partial x_i} \left( \frac{\partial U_i}{\partial x_i} + \frac{U_i}{\partial x_i} \right),$$  

It is clear that only viscous force and not pressure forces contribute to energy dissipation, now define the energy dissipation function $\Phi$ by

$$\Phi = \frac{\partial U_i}{\partial x_i} \left( \frac{\partial U_i}{\partial x_i} + \frac{\partial U_j}{\partial x_j} \right) = \frac{1}{2} \left( \frac{\partial U_i}{\partial x_i} + \frac{\partial U_j}{\partial x_j} \right)^2. \quad (2.38)$$

Which shows that $\Phi \geq 0$ and we have

$$\frac{dW}{dt} = \frac{1}{2} \frac{d}{dt} \left( U_j U_j \right) + \nu \Phi. \quad (2.39)$$

Similarly the heat transferred to the system from the surrounding is $Q$. We shall neglect the transfer of heat by radiation and consider only that by conduction. If we consider the element
of the volume, \( dv = dx dy dz \) of the mass \( \rho dv \), then the change in the total \( dE \) is equal to the change in the internal energy \( \rho dv e \) and a change in kinetic energy of an amount

\[
d \left[ \frac{1}{2} \rho dv \left( U_1^2 + U_2^2 + U_3^2 \right) \right],
\]

(2.40)
neglecting change in potential energy, we then have

\[
\frac{dE}{dt} = \rho dv \left\{ \frac{de}{dt} + \frac{1}{2} \frac{d}{dt} \left( U_1^2 + U_2^2 + U_3^2 \right) \right\}.
\]

(2.41)

where \( e \) is the thermal energy per unit mass.

### 2.3.3 Fourier Heat Conduction

This law states that the heat flux \( q \) per unit area is proportional to the temperature gradient, i.e.,

\[
q = \frac{1}{A} \frac{\partial Q}{\partial t} = -k \frac{\partial T}{\partial n}
\]

(2.42)
or,

\[
q = -k \nabla T, \text{ where } k \text{ is the thermal conductivity}
\]

The negative sign signifies that the heat flux is reckoned as positive in the direction of temperature gradient (i.e. heat flux in the direction of decreasing temperature). Hence the
amount of heat transferred into the volume $dv$ through the surface elements which are normal to the $x$ direction is equal to

$$\left(-k \frac{\partial T}{\partial n}\right) dydz,$$

(2.43)

The amount of heat leaving the volume is given by

$$\left[k \frac{\partial T}{\partial x} + \frac{\partial}{\partial x}\left(k \frac{\partial T}{\partial x}\right) dx\right] dydz,$$

(2.44)

Thus the amount of heat added by conduction in the $x$ direction during time $dt$ to volume $dv$ is

$$dt \cdot dv \frac{\partial}{\partial x}\left(k \frac{\partial T}{\partial x}\right),$$

(2.45)

Hence, the total amount of heat added in all directions is given by

$$\frac{\partial Q}{\partial t} = dv\left[\frac{\partial}{\partial x}\left(k \frac{\partial T}{\partial x}\right) + \frac{\partial}{\partial y}\left(k \frac{\partial T}{\partial y}\right) + \frac{\partial}{\partial z}\left(k \frac{\partial T}{\partial z}\right)\right],$$

(2.46)

Using equations (2.44) and (2.1.3.6), we obtain

$$\rho \frac{\partial e}{\partial t} = \frac{\partial}{\partial x}\left(k \frac{\partial T}{\partial x}\right) + \frac{\partial}{\partial y}\left(k \frac{\partial T}{\partial y}\right) + \frac{\partial}{\partial z}\left(k \frac{\partial T}{\partial z}\right) + \nu \Phi,$$

(2.47)

where,
\[
\Phi = 2 \left[ \left( \frac{\partial U_1}{\partial x} \right)^2 + \left( \frac{\partial U_2}{\partial y} \right)^2 + \left( \frac{\partial U_3}{\partial z} \right)^2 \right] + \left[ \frac{\partial U_1}{\partial y} + \frac{\partial U_2}{\partial x} \right]^2 + \left[ \frac{\partial U_3}{\partial x} + \frac{\partial U_1}{\partial z} \right]^2 + \left[ \frac{\partial U_3}{\partial y} + \frac{\partial U_2}{\partial z} \right]^2,
\]

Equation (2.47) holds for an incompressible fluid. For perfect fluid,

\[
\frac{de}{dt} = C_v \frac{dT}{dt}, \quad (de = C_v dT)
\]

(2.48)

Equation (2.47) now takes the form

\[
\rho C_v \frac{dT}{dt} = \nabla \cdot (k \nabla T) + \mu \Phi + H(T).
\]

(2.49)

where \( C_v \) is the specific heat at constant volume and \( H(t) \) is the heat source/sink term added to the equation depending whether it is positive or negative. From differential calculus, the left hand side of equation (2.49) can be written as:

\[
\rho C_v \frac{dT}{dt} = \rho C_v \left( \frac{dT}{dt} + (\vec{q} \cdot \nabla T) \right),
\]

(2.50)

where \( \vec{q} \) is the velocity vector.

Incorporating equation (2.50) into (2.49), we obtain the energy balance equation as

\[
\rho C_v \left( \frac{\partial T}{\partial t} + (\vec{q} \cdot \nabla)T \right) = \nabla \cdot (k \nabla T) + \mu \Phi + H(T).
\]

(2.51)
2.4 Concentration Equation

Mass transfer is another important concept in the field of chemical engineering and science in general. Mass transfer is the process responsible for the conversion of one component of species to another. In many systems, mass transfer process is made up of advection, diffusion and chemical kinetics. Advective transport is a function of the average linear velocity due to fluid flow. Diffusion is the macroscopic result of random thermal motion on a macroscopic scale. For example, in the diagram below, oxygen and nitrogen molecules move in random directions. If there are more oxygen molecules on the left side of the plane A-A than on the right, more molecules will cross to the right than the left: there will be a net flux even though the motion of each individual molecule is completely random.

Following the Fick’s Law, the flux is proportional to the gradient in concentration \((C)\) and is given by

\[
J = -DVC, \tag{2.52}
\]

where

- \(J\) = The mass flux. Flux is the movement of objects from one point to another in a given time. The flux is what we are measuring when studying diffusion.
- \(D\) = Mass Diffusivity. The diffusivity is the constant that describes how fast or slow an object diffuses.

The chemical kinetics can be the sum if sorption, desorption, decay, abiotic reaction and metabolism by bacteria. It may also be a function of multiple solutes. Moreover, the rate of chemical reaction typically kinetically limit mass transfer processes. Consider a given volume
in which mass transfer process takes place. The change in the number of molecules with time is the difference between the flux going in and the flux going out.

Using equation (2.52), the time rate of accumulation of chemical species in the volume is given as:

$$\frac{dC}{dt} = \nabla \cdot (D \nabla C) + R(C), \quad (2.53)$$

where $R(C)$ term in equation (2.53) represents the conversion of one component species to another by chemical kinetics. When $R(C)$ is negative, the reactant species is been consumed through the process. From differential calculus, the left hand side of equation (2.53) can be written as:

$$\frac{dC}{dt} = \frac{\partial C}{\partial t} + (\tau \cdot \nabla)C, \quad (2.54)$$

where $\tau$ is the velocity vector. Incorporating equation (2.53) into (2.54), we obtain the fundamental equation for advective-dispersive-reactive transport of chemicals and microbes as:

$$\frac{\partial C}{\partial t} + (\tau \cdot \nabla)C = \nabla \cdot (D \nabla C) + R(C), \quad (2.55)$$

Finally, the basic fluid equations to be investigated under some assumptions in the following chapters are as follows:
CONTINUITY EQUATION

\[ \frac{\partial \rho}{\partial t} + \vec{q} \cdot \nabla \rho = 0. \]

LINEAR MOMENTUM EQUATION

\[ \rho \left( \frac{\partial \vec{q}}{\partial t} + (\vec{q} \cdot \nabla)\vec{q} \right) = \nabla p + \nabla \cdot \sigma + \rho F. \]

ENERGY EQUATION

\[ \rho C_p \left( \frac{\partial T}{\partial t} + \vec{q} \cdot \nabla T \right) = \nabla \cdot (k \nabla T) + \mu \phi + H(T). \]

CHEMICAL SPECIES CONCENTRATION EQUATION

\[ \frac{\partial C}{\partial t} + (\vec{q} \cdot \nabla)C = \nabla \cdot (D \nabla C) + R(C). \]
3 Modelling boundary layer flow of a nanofluid past a permeable flat surface with Newtonian heating

3.1 Summary

The boundary layer stagnation point flow of a nanofluid past a permeable flat surface with Newtonian heating is studied. The model used for the nanofluid is the one which incorporates with the effects of Brownian motion and thermophoresis. The basic partial differential equations are reduced to an ordinary differential equation using similarity transformation approach. The model equations for the nanofluid velocity, temperature and nanoparticle concentration distributions depend on six parameters; Prandtl number $Pr$, Lewis number $Le$, Biot number $Bi$, the Brownian motion parameter $Nb$, the thermophoresis parameter $Nt$, and the suction/injection parameter $\beta$. The expressions for the local skin friction, local Nusselt number and the local Sherwood number are obtained and discussed.

3.2 Introduction

Conventional fluids, such as water, mineral oils, engine oil and ethylene glycol are normally used as heat transfer fluids and play an important role in many industry processes including
power generation, chemical processes, heating and cooling processes, transportation, microelectronics and other micro-sized applications. The poor heat transfer properties of these fluids constitute a limitation in improving the heat transfer augmentation and compactness of the heat exchangers.

Moreover, the use of solid particles as additive suspended into the base fluid is a technique for the heat transfer enhancement. The term nanofluid refers to a solid-liquid mixture with a continuous phase which is a nanometer sized particle dispersed in conventional base fluids. The particles are different from conventional particles (millimetre or micro-scale) in that they keep suspended in the fluid and no sedimentation occurs. Some numerical and experimental studies on nanofluids include thermal conductivity (Kang et al. [74]), separated flow (Abu-Nada [1]) and convective heat transfer (Khanafer et al. [80], Maiga et al. [109], Jou and Tzeng [72], Hwang et al. [66], Tiwari and Das [160], Oztop and Abu-Nada [129], Abu-Nada and Oztop [2] and Muthamilselvan et al. [124]). Daungthongsuk and Wongwises [33] studied the influence of thermophysical properties of nanofluids on the convective heat transfer and summarized various models used in literature for predicting the thermophysical properties of nanofluids. They analyzed the convective heat transfer coefficient in double-tube counter flow heat exchanger in the presence of TiO$_2$-water nanofluid. Studies on natural convection using nanofluids are very limited and they are related with differentially heated enclosures. Eastman et al. [41] used pure copper nanoparticle of less than 10nm sized and achieved 40% increase in thermal conductivity for only 0.3% volume fraction of the dispersed in ethylene glycol. They showed with some preliminary experiments with suspended nanoparticle, the conductivity of approximately 60% can be obtained with 5 vol. % CuO nanoparticles in the based fluid of water. Heat transfer coefficient is the determining

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factor in the forced convection cooling-heating applications of heat exchange equipments including engines and engine systems. Such enhancements mainly depend upon factors such as particle volume concentration, particle material, particle size, particle shape, base fluid material, temperature and additives. The comprehensive references on nanofluid can be found in the recent book by Das et al. [30] and the review papers by Daungthongsuk and Wongwisers [32], Trisaksri and Wongwise [161], Wang and Mujumdar [173], Kaka? and Pramanjaroenkij [73]. The principal aim of this dissertation is to study the mixed convention boundary layer flow past a vertical flat plate embedded in a porous medium filled with a nanofluid, the base fluid being water. Based on the literature survey only the papers by Nield and Kuznetsov [128] have extended the paper by Cheng and Minkowycz [24] on free convection boundary layer flow past a vertical flat plate embedded in a porous medium to the case when the porous medium is filled with a nanofluid. Nield and Kuznetsov [127] have also studied the classical problem of free convection boundary layer flow of a viscous and incompressible fluid (Newtonian fluid) past a vertical flat plate to the case of nanofluids. In both of these papers, the authors have used the nanofluid model proposed by Buongiorno [20]. Although this author discovered that seven slip mechanisms take place in convective transport in nanofluids, it is only the Brownian diffusion and the thermophoresis that are the most important when the turbulent flow effects are absent, Khan and Pop [79]. Meanwhile, Aziz [8] has previously used a convective boundary condition to study the Blassius flow over a flat plate. Following his paper, several authors have used the convective boundary condition to revisit the problems that were previously studied with the isothermal or the isoflux boundary conditions. A few examples are the papers by Bateller [11], Yao et al [197], Makinde and Aziz [112], and Makinde [110]. Moreover, it is interesting to note that studies related the influence of a convective boundary condition on the boundary layer flow of
nanofluids are still very scarce in the literature. In this chapter, a model of boundary layer stagnation point flow of nanofluids with heat and mass transfer characteristics over a permeable flat surface in the presence of Newtonian heating will be presented, analysed and discussed.

<table>
<thead>
<tr>
<th>Physical Property</th>
<th>base fluid (water)</th>
<th>Cu</th>
<th>Al₂O₃</th>
<th>TiO₂</th>
</tr>
</thead>
<tbody>
<tr>
<td>Cp(J/KgK)</td>
<td>4179</td>
<td>385</td>
<td>765</td>
<td>686.2</td>
</tr>
<tr>
<td>ρ (Kg/m³)</td>
<td>997.1</td>
<td>8933</td>
<td>3970</td>
<td>4250</td>
</tr>
<tr>
<td>k(W/mK)</td>
<td>0.613</td>
<td>400</td>
<td>40</td>
<td>8.9538</td>
</tr>
</tbody>
</table>

### 3.3 Convective transport equations.

Consider steady state two-dimensional boundary layer stagnation point flow of a nanofluid towards a permeable flat surface with a uniform suction velocity \( v_m = -V \) as shown in Figure 3.1 below:
The surface temperature $T_w$, to be determined later, is the result of a convective heating process which is characterised by a temperature $T_f$ and a heat transfer coefficient $h$. The nanoparticle volume fraction $C$ at the wall is $C_w$, while at large values of $y$, the value is $C_∞$. The Bougiorno [20] model may be modified for this problem to give the following continuity, momentum, energy and volume fraction equations

$$\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} = 0,$$

(3.1)

$$u \frac{\partial u}{\partial x} + v \frac{\partial u}{\partial y} = U_0 \frac{dU_0}{dx} + v \left( \frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} \right),$$

(3.2)

$$u \frac{\partial T}{\partial x} + v \frac{\partial T}{\partial y} = \alpha \left( \frac{\partial^2 T}{\partial x^2} + \frac{\partial^2 T}{\partial y^2} \right) + r \left[ D_f \left( \frac{\partial C}{\partial x} \frac{\partial T}{\partial x} + \frac{\partial C}{\partial y} \frac{\partial T}{\partial y} \right) + \frac{D_f}{T_∞} \left[ \left( \frac{\partial T}{\partial x} \right)^2 + \left( \frac{\partial T}{\partial y} \right)^2 \right] \right],$$

(3.3)
\[ u \frac{\partial C}{\partial x} + v \frac{\partial C}{\partial y} = D_B \left( \frac{\partial^2 C}{\partial x^2} + \frac{\partial^2 C}{\partial y^2} \right) + \frac{D_T}{T_w} \left( \frac{\partial^2 T}{\partial x^2} + \frac{\partial^2 T}{\partial y^2} \right), \]  

(3.4)

with boundary conditions at the surface:

\[ u = 0, \ v = V, \ C = C_w, \ -k \frac{\partial T}{\partial y} = h(T_f - T), \text{ at } y = 0. \]  

(3.5)

Far away from the wall i.e. as \( y \) tends to infinity:

\[ u = U_\infty (x), \ C = C_w, T = T_\infty \text{ as } y \to \infty, \]  

(3.6)

where \( u \) and \( v \) are the velocity components along the \( x \) and \( y \) directions respectively, \( p \) is the fluid pressure, \( \rho_f \) is the density of base fluid, \( \nu \) is the kinematic viscosity of the base fluid, \( \alpha \) is the thermal diffusivity of the base fluid, \( \tau = \left( \frac{\rho C_p}{\rho_f} \right)^\infty / \left( \frac{\rho C_p}{\rho_f} \right)_f \) is the ratio of nanoparticle heat capacity and the base fluid, \( D_B \) is the Brownian diffusion coefficient, \( D_T \) is the thermophoretic diffusion coefficient and \( T \) is the local temperature, \( V > 0 \) represents uniform suction, while \( V < 0 \) represents uniform injection. The case of \( V = 0 \) corresponds to impermeable plate surface. The subscript \( \infty \) denotes the free stream values at large values of \( y \) where the fluid is assumed to be accelerating with the velocity \( U_\infty (x) = ax \). We introduce the following dimensionless quantities

\[ \eta = y \sqrt{\frac{a}{\nu}}, \ \psi = (a \nu)^{1/2} x f (\eta), \ \theta = \frac{T - T_\infty}{T_f - T_\infty}, \ \phi = \frac{C - C_w}{C_w - C_x}. \]  

(3.7)

From equation (3.1),
\[
\frac{\partial}{\partial x} \left( \frac{\partial \psi}{\partial y} \right) + \frac{\partial}{\partial y} \left( - \frac{\partial \psi}{\partial x} \right) = 0.
\]

\[
\frac{\partial^2 \psi}{\partial x \partial y} - \frac{\partial^2 \psi}{\partial x \partial y} = 0. \quad (3.8)
\]

Hence the continuity equation is satisfied by

\[
v = -\frac{\partial \psi}{\partial x}, \quad u = \frac{\partial \psi}{\partial y}, \quad (3.9)
\]

now,

\[
\frac{\partial}{\partial x} = \frac{\partial}{\partial \eta} \frac{\partial \eta}{\partial x}, \quad \text{"and"} \quad \frac{\partial}{\partial y} = \frac{\partial}{\partial \eta} \frac{\partial \eta}{\partial y}, \quad (3.10)
\]

then,

\[
\frac{\partial \eta}{\partial y} = \sqrt{\frac{a}{\nu}}, \quad \frac{\partial \eta}{\partial x} = 0, \quad (3.11)
\]

\[
u = \frac{\partial \psi}{\partial x} = \frac{\partial \psi}{\partial \eta} \frac{\partial \eta}{\partial y} = \sqrt{\frac{a}{\nu}} \left( \frac{a}{\nu} \right)^{1/2} x f'(\eta),
\]

\[
u = \frac{\partial \psi}{\partial x} = - \left( \frac{a}{\nu} \right)^{1/2} f'(\eta), \quad (3.12)
\]

where prime symbol represent derivatives with respect to \( \eta \).

Now

\[
\frac{\partial u}{\partial y} = \frac{\partial u}{\partial \eta} \frac{\partial \eta}{\partial y}, \quad (3.13)
\]

Recall equation (3.11)
\[
\frac{\partial u}{\partial y} = \sqrt{\frac{a}{\nu}} (a\nu)^{\frac{1}{2}} x f''(\eta).
\]

(3.13)

\[
\frac{\partial^2 u}{\partial y^2} = \frac{\partial}{\partial \eta} \frac{\partial \eta}{\partial y} \left[ \sqrt{\frac{a}{\nu}} a x f''(\eta) \right].
\]

(3.14)

\[
\frac{\partial^2 u}{\partial y^2} = \frac{a^2 x}{\nu} f''''(\eta).
\]

Recall,

\[
U_\infty(x) = ax, \text{ then differentiating } U \text{ at } \infty \text{ with respect to } x
\]

\[
U_\infty \frac{dU_\infty}{dx} = ax \cdot a = a^2 x.
\]

(3.15)

Now substitute equations (3.13), (3.14) and (3.15) into equation (3.2)

where \[
\frac{\partial u}{\partial x} = a f''(\eta) \quad \text{and} \quad \frac{\partial^2 u}{\partial x^2} = 0
\]

(3.16)

\[
axf''(\eta) \frac{\partial}{\partial x} (axf''(\eta)) + (-a\nu)^{\frac{1}{2}} f(\eta) \sqrt{\frac{a}{\nu}} a x f''(\eta) = a^2 x + \nu^2 \frac{a^2 x}{\nu^2} f''''(\eta)
\]

\[
axf''(\eta)af''(\eta) - (a\nu)^{\frac{1}{2}} f(\eta) \sqrt{\frac{a}{\nu}} a x f''(\eta) = a^2 x + \nu^2 \frac{a^2 x}{\nu} f''''(\eta),
\]

(3.17)

cancelling \( \nu^2 \) and \( x \), then the equation below is derived,
\( f'' + ff' - f'^2 + 1 = 0. \) \hspace{1cm} (3.18)

Similarly,

\[
\frac{\partial T}{\partial x} = \frac{\partial T}{\partial \eta} \frac{\partial \eta}{\partial x} = 0, \quad \text{and} \quad \frac{\partial^2 T}{\partial x^2} = 0. \hspace{1cm} (3.19)
\]

\[
\frac{\partial T}{\partial y} = \frac{\partial T}{\partial \eta} \frac{\partial \eta}{\partial y}, \hspace{1cm} (3.20)
\]

but,

\[
T = (T_f - T_s) \theta + T_s. \hspace{1cm} (3.21)
\]

Recall equation (3.11),

therefore,

\[
\frac{\partial T}{\partial \eta} = \frac{\partial}{\partial \eta} (T_f - T_s) \theta' + T_s, \hspace{1cm} (3.22)
\]

\[
\frac{\partial T}{\partial \eta} = (T_f - T_s) \theta' (\eta). \hspace{1cm} (3.23)
\]

Recall equation (3.10),

therefore,

\[
\frac{\partial^2 T}{\partial y^2} \frac{\partial}{\partial y} = \frac{\partial}{\partial y} \sqrt{\frac{a}{u}} (T_f - T_s) \theta'(\eta). \hspace{1cm} (3.23)
\]
\[
\frac{\partial^2 T}{\partial y^2} = \frac{\partial}{\partial \eta} \sqrt{\frac{a}{\nu}} \frac{a}{\nu} (T_f - T_w) \phi'(\eta) = \frac{\partial}{\partial \eta} \sqrt{\frac{a}{\nu}} (T_f - T_w) \phi'(\eta),
\]

\[
\frac{\partial^2 T}{\partial y^2} = \frac{a}{\nu} (T_f - T_w) \phi''(\eta).
\]  
(3.24)

Similarly,

\[
\frac{\partial C}{\partial y} = \frac{\partial C}{\partial \eta} \frac{\partial \eta}{\partial y},
\]

but \( C = (C_w - C_x)\phi + C_x. \)  
(3.26)

\[
\frac{\partial C}{\partial \eta} = \frac{\partial}{\partial \eta} (C_w - C_x)\phi + C_x.
\]  
(3.27)

Therefore,

\[
\frac{\partial C}{\partial y} = \sqrt{\frac{a}{\nu}} \frac{\partial}{\partial \eta} ((C_w - C_x)\phi + C_x),
\]

\[
\frac{\partial C}{\partial y} = \sqrt{\frac{a}{\nu}} (C_w - C_x)\phi'(\eta).
\]  
(3.28)

Substitute equations (3.23), (3.24) and (3.28) into equation (3.3).

Recall equation (3.19)

\[
-(a \nu)^{\frac{1}{2}} f(\eta) \sqrt{\frac{a}{\nu}} (T_f - T_w) \phi''(\eta) = \alpha \frac{a}{\nu} (T_f - T_w) \phi''(\eta) + D_{\phi} \tau \sqrt{\frac{a}{\nu}} (C_w - C_x) \phi'(\eta) \sqrt{\frac{a}{\nu}} (T_f - T_w) \phi'(\eta)
\]

\[
+ \frac{D_{\phi}}{T_w} \left[ \sqrt{\frac{a}{\nu}} (T_f - T_w) \phi'(\eta) \right],
\]

(3.29)
\(-a\phi(\eta)\theta'(\eta) = \frac{a}{Pr} \phi'(\eta) + D_{B} \frac{\alpha}{\nu} (C_{w} - C_{\infty}) \phi' \theta'(\eta) + \frac{D_{r} a}{T_{w} \nu} (T_{f} - T_{w}) \theta'\eta), \)

\(-a\phi(\eta)\theta'(\eta) = \frac{a}{Pr} \phi'(\eta) + D_{B} \frac{\alpha}{\nu} (C_{w} - C_{\infty}) \phi' \theta'(\eta) + \frac{D_{r} a}{T_{w} \nu} (T_{f} - T_{w}) \theta'\eta), \)

after cancelling \(a\)

\[-f(\eta) \theta'(\eta) = 1 \frac{\theta'(\eta)}{Pr} + D_{B} \frac{\tau}{\nu} (C_{w} - C_{\infty}) \phi'(\eta) \theta'(\eta) + \frac{D_{r} a}{T_{w} \nu} (T_{f} - T_{w}) \theta'\eta. \tag{3.30} \]

But;

\[P_{r} = \frac{\nu}{\alpha}, \quad Nb = \tau \frac{D_{B}}{\nu} (C_{w} - C_{\infty}), \quad Nt = \frac{D_{r}}{T_{w} \nu} (T_{f} - T_{w}). \tag{3.31} \]

Then multiply through by \(Pr\) and substitute equation (3.31) into equation (3.30),

\[-Pr \phi'(\eta) = \theta''(\eta) + Pr Nb \phi'(\eta) \phi'(\eta) + Pr Nt \theta'\eta. \tag{3.32} \]

\[\theta'' + Pr Nb \phi' \theta' + Pr Nt \theta'\eta + Pr \theta = 0. \tag{3.33} \]

Finally,

\[\frac{\partial C}{\partial x} = \frac{\partial^{2} C}{\partial x^{2}} = 0. \tag{3.34} \]

\[\frac{\partial^{2} C}{\partial y^{2}} = \frac{\partial}{\partial y} \frac{\partial C}{\partial y}. \tag{3.35} \]

Recall from equation (3.28)
\[ \frac{\partial C}{\partial y} = \sqrt{\frac{a}{v}}(C_w - C_\infty) \phi', \quad (3.36) \]

also recall equation (3.10),
\[ \frac{\partial^2 C}{\partial y^2} = \frac{\partial}{\partial y} \left[ \sqrt{\frac{a}{v}}(C_w - C_\infty) \phi'(\eta) \right], \]
\[ \frac{\partial^2 C}{\partial y^2} = \frac{\partial}{\partial \eta} \frac{\partial \eta}{\partial y} \left[ \sqrt{\frac{a}{v}}(C_w - C_\infty) \phi'(\eta) \right] = \frac{\partial}{\partial \eta} \left[ \sqrt{\frac{a}{v}} \sqrt{\frac{a}{v}}(C_w - C_\infty) \phi'(\eta) \right], \]
\[ \frac{\partial^2 C}{\partial y^2} = \frac{a}{v}(C_w - C_\infty) \phi''(\eta). \quad (3.37) \]

Now substitute equations (3.24) and (3.26) into equation (3.4),
\[ - (av)^{1/2} f(\eta) \sqrt{\frac{a}{v}}(C_w - C_\infty) \phi'(\eta) = D_B \frac{a}{v}(C_w - C_\infty) \phi''(\eta) + \frac{D_r}{T_\infty} \left[ \frac{a}{v} (T_f - T_\infty) \theta''(\eta) \right], \]
\[ - f(\eta) \phi'(\eta) = D_B \frac{1}{v} \phi''(\eta) + \frac{D_r}{T_\infty} \left[ \frac{1}{(C_w - C_\infty)} (T_f - T_\infty) \theta''(\eta) \right]. \quad (3.38) \]

But,
\[ Le = \frac{v}{D_B}. \quad (3.39) \]

Therefore,
\[ \phi'' + Lef \phi' + \frac{Nt}{Nb} \theta'' = 0. \quad (3.40) \]
The basic model equations to solve are the following set of nonlinear ordinary differential equations:

\[ f''' + ff'' + f'^2 + 1 = 0. \quad (3.18) \]

\[ \theta'' + Pr f \theta' + Pr Nb \phi' \theta' + Pr Nt \theta'^2 = 0, \quad (3.33) \]

\[ \phi'' + Le f \phi' + \frac{Nt}{Nb} \theta'' = 0, \quad (3.40) \]

Subject to the following boundary conditions:

\[ f(0) = -\beta, \quad f'(0) = 0, \quad \theta'(0) = -Bi[1 - \theta(0)], \quad \phi(0) = 1; \quad (3.41) \]

\[ f'(\infty) = 1, \quad \theta(\infty) = 0, \quad \phi(\infty) = 0; \quad (3.42) \]

where primes denote differentiation with respect to \( \eta \) and the six parameters appearing in equations (3.31) and (3.39) are defined as follows:

\[ Pr = \frac{\nu}{\alpha}, \quad Le = \frac{\nu}{D_B}, \quad Nb = \frac{(\rho c)_p D_B (\phi_w - \phi_\infty)}{(\rho c)_f \nu T_\infty}, \]

\[ Nt = \frac{(\rho c)_p D_f (T_f - T_\infty)}{(\rho c)_f \nu T_\infty}, \quad Bi = \frac{h(\nu/a)^{1/2}}{k}, \quad \beta = \frac{V}{\sqrt{a \nu}}. \quad (3.43) \]

In equation (3.40), \( Pr \), \( Le \), \( Nb \), \( Nt \), \( Bi \), and \( \beta \) denote the Prandtl number, the Lewis number, the Brownian motion parameter, the thermophoresis parameter, Biot number and suction \( (\beta > 0) \)/ injection \( (\beta < 0) \) parameter, respectively.
3.4 Important Physical quantities.

The reduced Nusselt number $Nur$ and the Sherwood $Shr$ may be found in terms of the dimensionless temperature at the sheet surface, $\theta'(0)$ and the dimensionless concentration at the sheet surface, $\phi'(0)$, respectively i.e.

$$Nur = (Re_x)^{-\frac{1}{2}} Nu = -\theta'(0).$$

$$Shr = (Re_x)^{-\frac{1}{2}} Sh = -\phi'(0). \quad (3.44)$$

Where,

$$Nu = \frac{q_w x}{k(T_f - T_{\infty})}, \quad Sh = \frac{q_w x}{D_B (C_w - C_{\infty})}, \quad Re_x = \frac{U_x x}{v}, \quad q_w = -k \frac{\partial T}{\partial y} |_{y=0}, \quad \phi_m = -D_B \frac{\partial C}{\partial y} |_{y=0},$$

and $q_m$ is the surface heat flux and $q_w$ is the surface mass flux.

Skin friction is given as;

$$\tau_w = \frac{\partial u}{\partial y} |_{y=0}. \quad (3.46)$$

$$\frac{\partial u}{\partial y} = \frac{\partial}{\partial y} (axf') = \frac{\partial}{\partial \eta} (axf') \frac{\partial \eta}{\partial y},$$

$$= axf'' \frac{a^{\frac{1}{2}} x}{\nu^{\frac{1}{2}}} f''(\eta). \quad (3.47)$$
\[ C_f = \frac{\tau_w \nu^{1/2}}{a^{1/2} x} = f''|_{\eta=0} = f''(0). \]  

(3.48)

The above reduced Nusselt number and reduced Sherwood number are derived as follows;

Nusselt number (Heat transfer rate at the plate surface).

Recall equation (3.45),

where;

\[ q_w = -\frac{\partial T}{\partial \eta} \frac{\partial \eta}{\partial y} = -(T_f - T_\infty) \theta' \sqrt{\frac{a}{\nu}}. \]  

(3.48)

\[ Nu = -x \sqrt{\frac{a}{\nu}} \theta'(0) = \left(\frac{x a}{\nu} \right)^{1/2} \frac{1}{x} \theta'(0) = -\left(\frac{U_x x}{\nu} \right)^{1/2} \theta'(0), \]

\[ Nu = -\left(Re_x \right)^{1/2} \theta'(0). \]  

(3.49)

Therefore

\[ Nur = Re_x^{-1/2} \quad Nu = -\theta'(0). \]  

(3.50)

Similarly, recall from equation (3.45),

\[ Sh = \frac{q_m x}{C_w - C_w}. \]

Where,
\[ q_m = -\frac{\partial C}{\partial y} \bigg|_{y=0}, \]
\[ q_m = -\frac{\partial C}{\partial y} \frac{\partial \eta}{\partial y} = -(C_w - C_\infty) \phi' \sqrt{\frac{a}{\nu}}, \]

\[ Sh = -x \sqrt{\frac{a}{\nu}} \phi'(0) - \frac{(xa)^{\frac{1}{2}}}{\nu^{\frac{3}{2}}} = \left( \frac{U_x x}{\nu} \right)^{\frac{1}{2}} \phi'(0) = -Re^{\frac{1}{2}} \phi'(0), \] (3.51)

\[ Shr = Re^{\frac{1}{2}} Sh = -\phi'(0). \] (3.52)
4 Computational Analysis of the Model Problem

4.1 Summary

In this chapter, the set of nonlinear coupled ordinary differential equations together with their corresponding boundary conditions modelling the heat and mass transfer characteristics of a nanofluid stagnation point flow over a flat surface obtained in chapter 3 are solved numerically using Maple 12 which uses a fourth-fifth order Runge–kutta–Fehlberg algorithm together with shooting method for solving nonlinear boundary value problems. Numerical results are presented both in tabular and graphical forms illustrating the effects of these parameters on velocity, thermal and concentration boundary layers.

4.2 Numerical Procedure

In Chapter 3, we obtained the following set of nonlinear boundary value problems;

\[ f''' + f' - f''^2 + 1 = 0, \quad (3.18) \]

\[ \theta'' + Pr f \theta' + Pr Nb \phi' \theta' + Pr Nt \theta'^2 = 0, \quad (3.33) \]
\[
\phi'' + \beta \phi' + \frac{Nt}{Nb} \theta'' = 0, \tag{3.40}
\]

Subject to the following boundary conditions;

\[
f(0) = -\beta, \quad f'(0) = 0, \quad \theta'(0) = -B_i[1 - \theta(0)], \quad \phi(0) = 1, \tag{3.41}
\]

\[
f'(\infty) = 1, \quad \theta(\infty) = 0, \quad \phi(\infty) = 0. \tag{3.42}
\]

Equations (3.18), (3.33) and (3.40) together with the boundary conditions in equations (3.41) and (3.42) have been solved numerically using fourth-fifth order Runge-Kutta-Fehlberg algorithm together with shooting method implemented on Maple 12. The numerical procedure is as follows;

Let;

\[
f = x_1, \quad f' = x_2, \quad f'' = x_3, \quad \theta = x_4, \quad \theta' = x_5, \quad \phi = x_6, \quad \phi' = x_7. \tag{4.1}
\]

Equations (3.18), (3.33) and (3.40) are transformed into systems of first order differential equations as follows;

\[
x'_1 = x_2, \quad x'_2 = x_3, \quad x'_3 = x_2^2 - x_1 x_3, \quad x'_4 = x_5, \quad x'_5 = -Pr \, x_1 x_2 - Pr \, Nbx_7 x_5 - Pr \, Ntx_5^2, \quad x'_6 = x_7, \quad x'_7 = -Lex_1 x_7 + \frac{Nb}{Nt} (Pr x_1 x_5 + Pr Nbx_7 x_5 + Ntx_5^2),
\]

Subject to the following initial conditions;

\[
x_1(0) = -\beta, \quad x_2(0) = 0, \quad x_3(0) = 0, \quad x_4(0) = s_2,
\]

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In shooting method, the unspecified initial conditions \( s_1, s_2 \) and \( s_3 \) in equation (4.3) are assumed. Equation (4.2) is then integrated numerically as an initial valued problem to a given terminal point. The accuracy of the assumed missing initial condition is then checked by comparing the calculated value of the dependent variable at the terminal point with its given value there. If a difference exists, improved values of the missing initial conditions must be obtained and the process is repeated. The computations were done by a written program which was implemented on Maple. A step size of \( \Delta \eta = 0.001 \) was selected to be satisfactory for a convergence criterion of \( 10^{-7} \) in nearly all cases. The maximum value of \( \eta \) to each group of parameters \( Pr, Le, Nb, Nt, Bi \) and \( \beta \) is determined when the values of unknown boundary conditions at \( \eta = 0 \) did not change to successful loop with error with less than \( 10^{-7} \). From the process of numerical computation, the local skin friction coefficient, the reduced Nusselt number \( Nur \) and the reduced Sherwood number \( Shr \), which are respectively proportional to \( f''(0), -\theta(0) \) and \( -\phi'(0) \) are worked out and their numerical values presented in a tabular form. The accuracy of this numerical method was validated by direct comparison with the numerical results reported by Makinde and Aziz [112] for the boundary layer flow of a nanofluid past stretching sheet with a convective modelled as

\[
f'''' + ff'' - f'^2 + 1 = 0, \tag{3.18}
\]

\[
\theta'' + Pr f\theta' + Pr Nb\phi'\theta' + Pr Nt\theta'^2 = 0, \tag{3.33}
\]

\[
\phi'' + Le f\phi' + \frac{Nt}{Nb} \theta'' = 0, \tag{3.40}
\]
with

\[ f(0) = 0, \quad f'(0) = 1, \quad \theta'(0) = -Bi[1 - \theta(0)], \quad \phi(0) = 1, \]  
(3.41)

\[ f'(\infty) = 0, \quad \theta(\infty) = 0, \quad \phi(\infty) = 0, \]  
(3.42)

and a perfect agreement is observed as demonstrated in tables (4.1)-(4.3).

**Table 4.1:** Computations showing comparison with Makinde and Aziz [112] for Nur, Shr and the surface temperature \( \theta(0) \) with \( Nt = Nb = 0.5 \)

<table>
<thead>
<tr>
<th>Pr</th>
<th>Bi</th>
<th>Le</th>
<th>Nur Makinde &amp; Aziz [112]</th>
<th>Shr Makinde &amp; Aziz [112]</th>
<th>( \theta(0) ) Makinde &amp; Aziz [112]</th>
<th>Nur Present</th>
<th>Shr Present</th>
<th>( \theta(0) ) Present</th>
</tr>
</thead>
<tbody>
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<td>1</td>
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<td>0.0789</td>
<td>1.5477</td>
<td>0.2107</td>
<td>0.0789</td>
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<tr>
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<td>0.0570</td>
<td>3.4881</td>
<td>0.4296</td>
<td>0.0570</td>
<td>3.4881</td>
<td>0.4296</td>
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</table>
Table 4.2: Computations showing comparison with Makinde and Aziz [112] for Nur when \( \text{Le}=10, \text{Pr}=10, \text{Bi}=0.1 \)

<table>
<thead>
<tr>
<th>( Nt )</th>
<th>( \text{Nur} ) ( (\text{Nb}=0.1) ) Makinde &amp; Aziz [112]</th>
<th>( \text{Nur} ) ( (\text{Nb}=0.2) ) Makinde &amp; Aziz [112]</th>
<th>( \text{Nur} ) ( (\text{Nb}=0.3) ) Makinde &amp; Aziz [112]</th>
<th>( \text{Nur} ) ( (\text{Nb}=0.1) ) Present</th>
<th>( \text{Nur} ) ( (\text{Nb}=0.2) ) Present</th>
<th>( \text{Nur} ) ( (\text{Nb}=0.3) ) Present</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.1</td>
<td>0.0929</td>
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<td>0.0769</td>
<td>0.0929</td>
<td>0.0873</td>
<td>0.0769</td>
</tr>
<tr>
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<td>0.0868</td>
<td>0.0751</td>
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<td>0.0751</td>
</tr>
<tr>
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</tr>
<tr>
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<td>0.0700</td>
<td>0.0921</td>
<td>0.0845</td>
<td>0.0700</td>
</tr>
</tbody>
</table>

Table 4.3: Computations showing comparison with Makinde and Aziz [112] for Shr when \( \text{Le}=10, \text{Pr}=10, \text{Bi}=0.1 \)

<table>
<thead>
<tr>
<th>( Nt )</th>
<th>( \text{Shr} ) ( (\text{Nb}=0.1) ) Makinde &amp; Aziz [112]</th>
<th>( \text{Shr} ) ( (\text{Nb}=0.2) ) Makinde &amp; Aziz [112]</th>
<th>( \text{Shr} ) ( (\text{Nb}=0.3) ) Makinde &amp; Aziz [112]</th>
<th>( \text{Shr} ) ( (\text{Nb}=0.1) ) Present</th>
<th>( \text{Shr} ) ( (\text{Nb}=0.2) ) Present</th>
<th>( \text{Shr} ) ( (\text{Nb}=0.3) ) Present</th>
<th>( \text{Nur} ) ( (\text{Nb}=0.1) ) Present</th>
<th>( \text{Nur} ) ( (\text{Nb}=0.2) ) Present</th>
<th>( \text{Nur} ) ( (\text{Nb}=0.3) ) Present</th>
</tr>
</thead>
<tbody>
<tr>
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<td>2.3109</td>
<td>2.3299</td>
<td>2.2774</td>
<td>2.3109</td>
<td>2.3299</td>
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<td>2.3299</td>
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</tr>
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<td>2.3570</td>
<td>2.4792</td>
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</tr>
</tbody>
</table>

4.3 Graphical Results

The numerical computations of the results are demonstrated in the Figures 4.1-4.17 below. In order to have greater insight in the qualitative analysis of the results, we have taken the values of various parameters controlling the flow systems as \( 1= \text{Pr}=10, -0.3= \beta = 1, 5= \text{Le}= 20, 0.1= \text{Bi}= 10, 0.1= \text{Nt}=0.5 \) and \( 0.1= \text{Nb}=0.5 \)

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Figure 4.1: Effect of suction/injection parameter on the velocity profiles when $Le=5$, $Pr=5$, $Bi=Nt=Nb=0.1$.

Figure 4.2: Effect of suction/injection parameter on the temperature profiles when $Le=5$, $Pr=5$, $Bi=Nt=Nb=0.1$.

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Figure 4.3: Effect of suction/injection parameter on the concentration profiles when $Le=5$, $Pr=5$, $Bi=Nt=Nb=0.1$

Figure 4.4: Effect of $Le$ on the temperature profiles when $Pr=5$, $\beta=Bi=Nt=Nb=0.1$

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Figure 4.5: Effect of Le on the concentration profiles when Pr=5, β=Bi=Nt=Nb=0.1

Figure 4.6: Effect of Nt and Nb on the temperature profiles when Le=Pr=5, β=Bi=0.1

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Figure 4.7: Effect of $N_t$ and $N_b$ on the concentration profiles when $\text{Le}=\text{Pr}=5, \beta=\text{Bi}=0.1$

Figure 4.8: Effect of $\text{Bi}$ on the temperature profiles when $\text{Le}=\text{Pr}=5, N_t=N_b=\beta=0.1$
Figure 4.9: Effect of Bi on the concentration profiles when Le=Pr=5, Nt= Nb=β=0.1

Figure 4.10: Effect of Pr on the temperature profiles when Le=5, Bi=Nt =Nb=β=0.1

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Figure 4.11: Effect of suction / injection parameter $\beta$ on the skin friction.

Figure 4.12: Effect of $N_i$ and $N_b$ on the reduced Nusselt number when $Pr=Le=5$, $Bi=\beta=0.1$
**Figure 4.13:** Effect of $N_t$ and $N_b$ on the reduced Sherwood number when $Pr=Le=5$, $Bi=\beta=0.1$

**Figure 4.14:** Effect of $Bi$ and $\beta$ on the reduced Nusselt number when $Pr=Le=5$, $N_t=N_b=0.1$
Figure 4.15: Effect of $Bi$ and $\beta$ on the reduced Sherwood number when $Pr=Le=5$, $Nt=Nb=0.1$

Figure 4.16: Effect of $Le$ on the reduced Sherwood number when $Pr=5$, $\beta=Bi=Nb=0.1$
Figure 4.17: Effect of Pr on the reduced Nusselt number when Le=5, β=Bi=Nb=0.1

Detail discussion on the graphical results outlined in section 4.3 will be presented in the following Chapter.
5.1 Analysis and discussion of the results

The numerical computations of the results are demonstrated in the Figures 4.1-4.17 and Tables 1-3 in chapter 4. In order to have greater insight in the qualitative analysis of the results, the values of various parameters controlling the flow systems as \( Pr = 10, -0.3 = \beta, 5 = Le = 20, 0.1 = Bi = 10, 0.1 = Nt = 0.5 \) and \( 0.1 = Nb = 0.5 \) have been taken. As a further check on the accuracy of the numerical computations of this work, the results of this work are being compared with that of Makinde and Aziz [112] in Tables 4.1-4.3 and an excellent agreement is established. In this chapter, the graphical results that provide additional insights into the problem under consideration is discussed.

5.2 Discussion of the tables

Table 4.1 contains the comparison with Makinde and Aziz [112] for reduced Nusselt number \( (Nur) \), reduced Sherwood number \( (Shr) \) and the surface temperature \( (\theta(0)) \) with thermophoresis parameter (i.e, the rate of heat transfer by the nanoparticle) and Brownian motion parameter (i.e, the rate of Brownian motion) \( 0.5 (Nt \leq Nb \leq 0.5) \) given as and varying Prandtl number, Lewis number and Biot number. It is clearly seen from the table that
as Prandtl number $Pr$ increases from 1 to 2, it enhances reduced Nusselt number (heat transfer rate) and the reduced Sherwood number (mass transfer rate) while the surface wall temperature reduces. It is interesting to note that as Prandtl number increases from 5 to 10, the heat transfer rate decreases while the mass transfer rate and the surface wall temperature were enhanced. As expected, when the rate of convective heat transfer ($Bi$) was increased, enhances the rate of heat transfer at the wall and the surface wall temperature while reduces the rate of mass transfer at the wall surface. Furthermore, as we increase the Lewis number, the rate of heat and mass transfer reduces while it enhances the wall surface temperature as expected.

Table 4.2 shows the comparison with Makinde and Aziz[112] for reduced Nusselt number when Lewis number, Prandtl number and the Biot number is given as 10, 10 and 0.1. It was noted that as we increase the thermophoresis and kept the Brownian motion, it was established that the heat transfer rate reduces but the highest values was observed when the Brownian motion $Nb$ is 10.

Table 4.3 contains the comparison with Makinde and Aziz [112] for reduced Sherwood number when Lewis and Prandtl numbers are given as 10 and Biot number is 0.1. The same values of the thermophoresis $Nt$ and Brownian motion $Nb$ was used. As the thermophoresis parameter increases, the rate of mass transfer reduces for $Nb = 0.1$, while for $Nb = 0.2$ and $0.3$, it enhances the mass transfer rate. It was interesting to note that the maximum values were obtained for $Nb = 0.3$ different from Table 4.2.2.
5.3 Discussion of the graphs

The samples of velocity, temperature and the nanoparticle volume fraction profiles are given in Figures 4.1-4.17, respectively. These profiles satisfy the far field boundary conditions (4.12-4.13) asymptotically, which support the numerical results obtained.

Figure 4.1 shows the effect of suction/injection parameter $\beta$ on the velocity profile. For suction, as $\beta$ increases, the boundary layer thickness increases and as for injection, the velocity boundary layer thickness reduces and thins out. This implies that as suction parameter is been increased, the rate of heat transfer is been enhanced and reduces the surface wall temperature.

Figure 4.2 describes the effect of suction/injection parameter on the temperature profile such that as suction parameter is increased, the thermal boundary layer decreases, as injection increases, the thermal boundary layer increases. This implies that convective transfer of heat between the cold fluid (i.e. nanofluid) on top of the surface and the hot fluid (ordinary fluid) below the permeable surface brings about a gradual decrease in temperature of the hot fluid as the cold fluid is being sucked down through the surface, while the temperature increases at the top of the surface as the hot fluid is being injected up to the cold fluid through the surface.

The rate of heat transfer also is enhanced but reduces the wall surface temperature.

Figure 4.3 shows the effect of suction/injection parameter on the concentration profile, as suction parameter increases, concentration boundary layer thickness decreases while as injection increases; the concentration boundary layer thickness thickens across the wall plate.

This explains that concentration is lower when the cold fluid flows down through the surface.
to the hot fluid but higher concentration is observed as the hot fluid flows up to the surface top and becomes cold.

Figure 4.4 shows the effect of Lewis number on temperature profile such that as the Lewis number increases, the thickness of the thermal boundary layer increases only at the wall of the plate. This indicates that as the rate of thermal diffusivity of the fluid increases due to the nanoparticles, the temperature at the surface also increases. An increase in Lewis number causes the reduced Nusselt number to decrease but enhances the reduced Sherwood number and the surface temperature.

Figure 4.5 discusses the significant effect of the Lewis number on concentration distribution. As the Lewis number increases, the volume fraction boundary layer thickness thins out across the wall plate. It implies that as the thermal diffusivity of the fluid increases, which also increases the temperature of the surface, the concentration of the fluid becomes very low. Also, the rate of mass transfer at the wall surface is enhanced and the concentration across the wall surface plate is reduced.

Figure 4.6 shows temperature distribution in the thermal boundary layer for different values of the Brownian motion and the thermophoresis parameter. As both Nb and Nt increase, the boundary layer thickness increases, as noted earlier in discussing the tabular data, the surface temperature increases, and the curves become less steep indicating a diminution of the reduced Nusselt number.
Figure 4.7 shows the curve of concentration profile against the coordinate $\eta$ for various values of the rate of Brownian motion $N_b$ and thermophoresis $N_t$ parameters. From the figure, it was observed that as the thermophoresis and Brownian motion parameters increases, significant increase in concentration boundary layer thickness away from the wall plate is observed.

Figure 4.8 shows the effect of Biot number on the thermal boundary layer which indicates that as it increases; the thermal boundary layer thickness increases across the plate. This implies that convective heat transfer is enhanced as convective heat transfer coefficient increases, which also increases the thermal penetration as expected.

In figure 4.9, because of the concentration distribution which is driven by the temperature field, it is suggested that an increase in Biot number, i.e the convective heat transfer coefficient, increases the rate of penetration of the concentration. Which implies that as the Biot number increases, the concentration increases as well.

Figure 4.10 represents the effect of Prandtl number on thermal boundary layer thickness as it increases. The thermal boundary layer thickness decreases as the curves become increasingly steeper. As a result of this, the reduced Nusselt number, being proportional to the initial slope, increases. This pattern is reminiscent of the free convective boundary layer flow in a regular fluid.

Figure 4.11 represents the effect of suction/injection on the skin-friction. From the graph, it is noted that suction/injection has no influence on the skin-friction coefficient. It is clearly
seen that as suction parameter increases across the plate the skin-friction coefficient increases. Similarly as injection increases, the skin-friction decreases across the plate.

Figure 4.12 shows the effect of the Brownian motion parameter and the thermophoresis parameter on the reduced Nusselt number. As the Brownian motion parameter increases, the thermal boundary layer increases leading to a decrease in the rate of heat transfer. Also as the thermophoresis parameter increases, the fluid temperature decreases leading to an increase in the heat transfer rate at across the plate surface.

Figure 4.13 shows the effect of Brownian motion parameter and the thermophoresis parameter for reduced Sherwood number. As the Brownian motion parameter increases from 0.1 to 0.2, the rate of mass transfer decreases across the wall plate as thermophoresis parameter increases. It is interesting to note that as the Brownian motion parameter increases from 0.3 to 0.35, the mass transfer rate across the wall plate increases. As the thermophoresis parameter increases, the fluid concentration decreases to an increase in the mass transfer rate across the plate surface.

Figure 4.14 shows the effect of suction/injection and Biot number on reduced Nusselt number. As the suction parameter increases, the rate of heat transfer increases across the wall plate and the convective heat transfer (Biot number) also increases. Similarly for injection parameter, reverse was the case. Also as the Biot number increases, the fluid temperature increases leading to a decrease in the heat transfer rate across the plate surface.
Figure 4.15 shows the effect of the suction/injection parameter and the Biot number on the reduced Sherwood number. As suction parameter is increasing, the rate of mass transfer increases across the wall plate increases. As injection parameter increases, the mass transfer rate across the wall plate decreases and the convective transfer rate is increased. It is interesting to note that for each values of suction/injection parameter used, the mass transfer rate decreases across the wall plate. And the convective heat transfer rate increases across the wall plate.

Figure 4.16 shows the effect of Lewis number and the thermophoresis parameter on the reduced Sherwood number. As the Lewis number increases, the rate of mass transfer increases across the wall plate as the thermophoresis parameter increases. It is interesting to note that as the Lewis number increases, the mass transfer rate across the wall plate increases. And as the thermophoresis parameter increases, the fluid concentration decreases to an increase in the mass transfer rate across the plate surface.

Figure 4.17 shows the effect of Prandtl number and thermophoresis parameter on the reduced Nusselt. As the Prandtl number increases, the thermal boundary layers decreases leading to an increase in the rate of heat transfer. Also as the thermophoresis parameter increases, the fluid temperature increases leading to a decrease in the heat transfer rate across the plate surface.
5.4 Conclusions

We examined the theoretical analysis of boundary layer flow of nanofluid with the characteristics of heat and mass transfer with suction/injection. The governing momentum, energy and concentration equations are solved using the fourth-fifth order of Runge-Kutta method alongside with shooting iteration scheme and our results show that the local skin friction, heat transfer rate and the mass transfer rate were affected by the embedded flow parameters. It is interesting to note that as Brownian motion parameter increases, the mass transfer rate decreases. Similarly, increasing the suction parameter increases the heat transfer rate and the convective heat transfer. It is noteworthy to mention that as the Lewis number increases, the mass transfer rate (Sherwood number) and the thermophoresis parameter increases across the wall plate. Enhanced Prandtl number decreases the thermal boundary layer thickness across the wall plate.
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