

**DETERMINATION OF THE GAS-FLOW PATTERNS INSIDE THE HOT-
WIRE CHEMICAL VAPOR DEPOSITION SYSTEM, USING A
COMPUTATIONAL FLUID DYNAMICS SOFTWARE (FLUENT)**

By

Thobeka Wittes



A thesis submitted in partial fulfillment of the requirements for the degree of Magister Scientiae in the Department of Physics, University of the Western Cape.

Supervisor:

Prof. D. Knoesen

Dept. of Physics

University of Western Cape

July 2009

DECLARATION

I, the undersigned, hereby declare that the work contained in this thesis is my own original work and that I have not previously in its entirety or in part submitted it at any university for a degree

Signature:

Date:.....



**DETERMINATION OF THE GAS-FLOW PATTERNS INSIDE THE HOT-
WIRE CHEMICAL VAPOR DEPOSITION SYSTEM, USING A
COMPUTATIONAL FLUID DYNAMICS SOFTWARE (FLUENT)**

BY

THOBEKA VICTORIA WITTES

KEYWORDS

CFD

HWCVD

Gas flow

Silane

Hydrogen



ABSTRACT

Computational Fluid Dynamics is the analysis of a system involving fluid flow, heat transfer and associated phenomena such as chemical reactions by means of a computer-based simulation. The simulations in this study are performed using (CFD) software package FLUENT. The mixture of two gases (Silane gas (SiH_4) and Hydrogen gas (H_2)) are delivered into the hot-wire chemical vapor deposition system (HWCVD) with the two deposited substrates (glass and Silicon). This process is performed by the solar cells group of the Physics department at the University of the Western Cape. In this thesis, the simulation is done using a CFD software package FLUENT, to model the gas-flow patterns inside the HWCVD system. This will show how the gas-flow patterns are affected by the varying temperature of the heater in each simulation performed in this study under a constant pressure of $60\mu\text{Bar}$ of the system.

ACKNOWLEDGEMENTS

Firstly I would like to thank God Almighty who kept me up until this far, guiding me and giving me strength, knowledge and wisdom and love to succeed. Above all, I thank God for who he is in my life.

I am truly thankful to the following people for their contribution towards making this thesis possible:-

- ❖ To my parents, for allowing me the opportunity of finishing my studies, and their continuous support and prayers throughout this study.
- ❖ Prof. Dirk Knoesen (University of the Western Cape), supervisor, for his continuous guidance and support throughout this study.
- ❖ Mr. Ian Schroeder (University of the Western Cape), for valuable guidance and support throughout this study.
- ❖ My precious family, amaHlotshane, oHala, Sophico, Yemyem, Qholomsila, Vela-baMbhentsele, words cannot explain how I feel about you guys. Ke Modimo fela a itseng, mara e, keya lona.
- ❖ uLonwabo-lwam Wittes, my boy I thank God every time I remember you “Philippians 1:3”, you have given me a reason to live and to look forward to the next day of my life.
- ❖ To Nombulelo Agnes Mthembu and her husband. Mmangwane Modimo a go hlogonolofatse le lelapa la gago ka moyo o montle and for planting this seed.

- ❖ Nathan Zhou, Tshepo Samuel Dinoko and Stephan Smittch for constant support and guidance throughout this study and the background of CFD, may the good Lord do you good.
- ❖ Mr. and Mrs. Maleka for your continuous guidance and support throughout this study, and letting us into your office.
- ❖ To my friends, Promise Tlhologelo Maredi, Steven Solethu Nkosi, Takalani Madima, Nombulelo Agnes Khwaza, Thato Tshabalala, for their moral support they provided throughout this study.
- ❖ To my precious four sisters and brother, Nongetheni Rosina, Lumkile Phillip, Nomthandazo Florence, Tombi Evelyn, Sindiswa Mildred Wittes for their continuous prayers, moral support, patience and guidance throughout this study.
- ❖ To Khwaza's family for your prayers and initiating my success may the good Lord increase the gift that he has given to you.
- ❖ To my home church, the Christian Apostolic Church in Zion of South Africa (Lichtenburg District); for starting this journey of my success. May the good Lord do you good.
- ❖ I cannot stop thanking my parents, Nozizwe Elizabeth and Vuyo Petrus Wittes for their prayers and love throughout my life. May the good Lord bless you and keep you for me.
- ❖ University of the Western Cape (UWC), iThemba LABS and the National Research Foundation (NRF) for both financial and moral support throughout this study and, lastly to my friends and those I have come into contact with over this study for their constant motivation.



To my family: Vuyo (Dad), Nozizwe (Mom),
Nongetheni, Lumkile, Nomthandazo,
Tombi, Sindiswa, Zolani,
Dumisani, Unathi, Mpendulo
no Lonwabo **Wittes**.

LIST OF FIGURES

Figure 1: The hot-wire chemical vapor deposition system used at the Physics department of the University of the Western Cape.	8
Figure 2.1: Schematic cross-section of HWCVD system.	12
Figure 2.2: A domain (geometry) of HWCVD system as used in this study, designed using Gambit.	17
Figure 2.3: A grid/mesh of the geometry of the HWCVD system.	18
Figure 3.1: A flow chart of the procedure followed in a CFD problem.	27
Figure 3.2: A domain of the gas-inlet pipes	29
Figure 3.3: A domain of the filaments, insulators and filaments stand.	30
Figure 3.4: Deposition chamber (CVD) with all the parts imported to it.	30
Figure 3.5: A grid/mesh of CVD system, with the total number of 657120 cells.	33
Figure 3.6: An overview of the segregated solution method when iterating.	38
Figure B1: Temperature contours.	60
Figure B2: Temperature contours with a plane drawn at ($y_0=-15$, $y_1=15$, $y_2=15$) axis.	61
Figure B3: Pathlines colored by the temperature.	62
Figure B4: Pathlines colored by the velocity.	63

LIST OF TABLES

Table 3.1: Some of the measurements of HWCVD system.	28
Table 3.2: The general data of the HWCVD system.	34
Table 3.3: Boundary conditions of HWCVD.	35
Table 3.4: Material properties used in this study.	36
Table 4.1: Mass flow-rate results for all simulations.	41
Table 4.2: Surface deposition-rate results for all simulations.	45
Table A1: A detailed CFD model used in this study.	55

LIST OF GRAPHS



Graph 4.1: A plot of the mass flow-rate on the filaments, inlets, outlet and two substrates vs. temperature of the heater for all simulations.	42
Graph 4.2: A plot of the net mass flow-rate results around the filaments, inlet , outlet and the two substrates vs. temperature of the heater.	43
Graph 4.3: A plot of the surface deposition-rate on the filaments, the two substrates and substrate-holder vs. temperatures of the heater.	46

NOMENCLATURE

Symbols:

Variable	Description	Unit
x	: distance in the x-direction	-
y	: distance in the y-direction	-
z	: distance in the z-direction	-
u	: velocity in the x-direction	m/s
v	: velocity in the y-direction	m/s
w	: velocity in the z-direction	m/s
t	: time	s
ρ	: density	kg/m ³
Pr	: Prandtl number	-
q	: heat flux	Wm ⁻²
Sc_{cm}	: standard cubic centimeter per minute	-
τ	: stress	N/m ²
μ	: dynamic molecular viscosity	kgm ⁻¹ s ⁻¹
δ_{ij}	: kronecker delta function	-
λ	: bulk viscosity	m/s ²
μ	: kinematics viscosity	m ² /s
V	: velocity vector	m/s
T	: temperature	K
S_m	: mass source	kg/m ³ -s
p	: pressure	Pa
$\dot{\Gamma}$: exchange coefficient (laminar + Turbulent)	-



C_p	: specific heat at constant pressure	J/kg-k
g	: gravitational acceleration	m/s ²
K	: thermal conductivity	W/m-k
D/D_t	: substantial derivative	-
ϕ	: dependent variable	-

Abbreviations:

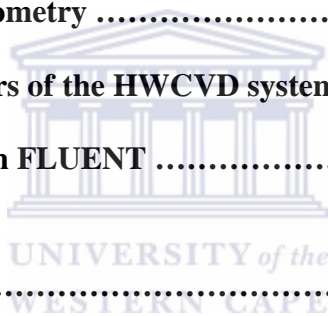
CFD	Computational Fluid Dynamics
HWCVD	Hot-wire Chemical Vapor Deposition System



CONTENTS

<i>KEYWORDS</i>	<i>i</i>
<i>ABSTRACT</i>	<i>ii</i>
<i>ACKNOWLEDGEMENT</i>	<i>iii</i>
<i>LIST OF FIGURES</i>	<i>vi</i>
<i>LIST OF TABLES</i>	<i>vii</i>
<i>LIST OF GRAPHS</i>	<i>vii</i>
<i>NOMENCLATURE</i>	<i>viii</i>
CHAPTER 1	1
Introduction	1
1.1 Background	1
1.2 Computational Fluid Dynamics	2
1.2.1 The CAD design (Gambit)	4
1.2.2 Solver	5
1.2.3 Post-processor	7
1.3 Hot-wire Chemical vapor deposition system	7
1.4 The Aim and Outline of this study	9
CHAPTER 2	11
Techniques used in this study	11
2.1 HWCVD	11
2.1.1 Background	11
2.1.2 HWCVD Process	13
2.2 Background on Gambit (CAD design)	15
2.3 Mesh Generation	16
2.4 Background on FLUENT	18

2.5 Finite Volume Methods	19
2.6 Mathematics behind CFD	20
2.6.1 Navier-Stokes equations	20
2.6.1.1 Conservation of Mass	21
2.6.1.2 Momentum equations	22
2.6.1.3 Energy equations	23
2.7 Steady state conditions and computational accuracy in FLUENT	24
<i>CHAPTER 3</i>	26
SIMULATION METHODS	26
3.1 Simulation Methods	26
3.2 Designing the domain/geometry	27
3.3 The deposition parameters of the HWCVD system	33
3.4 Starting the Simulation in FLUENT	35
<i>CHAPTER 4</i>	39
4. RESULTS AND DISCUSSIONS	39
4.1 Introduction	39
4.2 Mass flow-rate	40
4.3 Surface Deposition-rate	44
4.4 Discussions	47
<i>CHAPTER 5</i>	48
5. SUMMARY AND CONCLUSION	48
References	50
APPENDICES	54



Appendix A54

A.1 Introduction54

A.2 Calculation of the magnitude of inlet velocity56

A.3 Calculations of the heat flux of the filaments56

A.4 Species Mass Fraction57

Appendix B59

B.1 Contours and Path-lines59



CHAPTER 1

INTRODUCTION

1.1 Background

In this study we will use the Computational Fluid Dynamics (CFD) software FLUENT to model the gas flow patterns inside the Hot-wire chemical vapor deposition system (HWCVD), by designing the internal geometry of the HWCVD; using the FLUENT CAD design system GAMBIT.

The CFD software (FLUENT) is divided into three steps; namely [1, 13]:

- Pre-processor stage (which is the computer-aided design (CAD) software package Gambit) where the modeling goals are defined (in this study to model the gas-flow patterns inside the hot-wire chemical vapor deposition system, using the CFD software FLUENT), the domain to be modeled is identified/designed (the HWCVD system), finally design and create a grid/mesh from the geometry/domain designed.
- Solver stage, where the numerical model is set, then computes and monitor the solution.
- Post-processor stage, where the results are examined and if the results are not satisfying then consider revision to the model.

1.2 *Computational Fluid Dynamics*

CFD is the analysis of a system involving fluid flow, heat transfer and associated phenomena such as chemical reactions by means of computer-based simulation. The CFD is also a numerical modeling technique that solves the Navier-Stokes equations on a discretised domain of the geometry of interest with the appropriate flow boundary conditions supplied. The Navier-Stokes equations are a complex non-linear set of partial differential equations that describes the mass and momentum conservation of a fluid [1, 13].

From the 1960s onwards the aerospace industry has integrated the CFD technique into the design, research and development of the manufacturing of aircraft and jet engines. More recently the methods have been applied to the design of internal combustion engines, combustion chambers of gas turbines and furnaces. Furthermore, motor vehicle manufactures now routinely predict drag forces, under-bonnet air flows and the in-car environment with CFD. Increasingly CFD is becoming a vital component in the design of industrial products and process [1, 13].

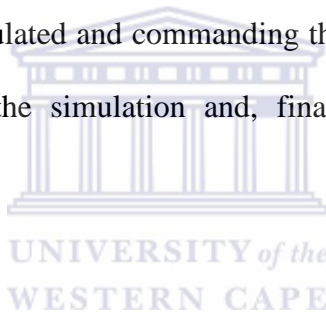
The aim of developments in the CFD field is to provide a capability comparable to other computer-aided engineering tools such as stress analysis codes.

There are several unique advantages of CFD over experimental-based approaches to fluid systems design which are given below [1, 13]:

- Substantial reduction of lead times and cost of new designs.
- Ability to study systems where controlled experiments are difficult or impossible to perform (e.g. very large systems).

- Ability to study systems under hazardous (dangerous) conditions at and beyond their normal performance limits (e.g. safety studies and accident scenarios).
- Practically unlimited level of detail of results.

The CFD code (FLUENT) has three basic components: the pre-processor, solver and the post-processor. The solver is the heart of the code; carrying out the major computations and providing the numerical solutions. The pre-processor and the post-processor are the front and the end of the code, providing the user/machine interface that allows a CFD operator to communicate with the solver: by inputting data to define the problem to be simulated and commanding the solver to use certain models and schemes to carry out the simulation and, finally, presenting for study the computed results [1, 13].



Apart from these key elements, a commercial package aimed at multi-purpose modeling will have a suite of models for various flow problems, such as various turbulence models to cover a range of turbulence conditions and assumptions. The CFD package also has a library of material properties for defining the fluid media and solid boundaries in the computational domain [1].

1.2.1 The CAD design (GAMBIT)

Drafting in a CAD design can be done in two dimensions (2D) or three dimensions (3D). In this study the drafting of the internal geometry of the HWCVD system was done in 3D. With this the system is represented by three projected views at right angles. This allows rotations in three dimensions, allowing viewing of a design from any desired angle, even from the inside looking out [9].

The CAD design which was used in this study is GAMBIT (Geometry and Mesh Building Intelligent Toolkit). It has a number of functions that allows the user to define a fluid domain, known as the computational domain, and build up the physical geometry of the zone considered, creating mesh/grid system throughout the domain and tuning this mesh to improve computation quality, including accuracy and speed. The user may also specify the properties of the fluid and other materials in contact with the fluid at this stage [1, 9].

The pre-processor (GAMBIT) allows the user to define the fluid flow phenomena to be modeled, to choose from the appropriate physical or chemical models provided by the package, and to select the numerical parameters and initial and boundary conditions for the computation. All these features are crucial in ensuring a quality CFD modeling task [9].

For example, the mesh/grid refinement at this stage (GAMBIT) affects directly the accuracy of the solution and the cost of computation, in terms of computation time

and hardware requirement. An optimized mesh/grid system uses less computer memory space, requires less computing, and yet gives satisfactory accuracy [1, 9].

1.2.2 Solver

As mentioned above, the solver stage is the heart of a CFD code. It is a collection of various algorithms and numerical techniques that performs the major computation task described in the pre-processor above. It consists of two components that provide a discretization for the defining equations and subsequent (resultant) solution [1, 9].

The first component uses a discretizing scheme to express the governing equations in a discretized form for all mesh/grid elements over the whole computational domain and discretizes the boundary equations appropriate at the boundary elements. In summary, this section converts the partial differential equations and boundary conditions formulae into a group of algebraic equations. The second part uses an iterative procedure to find solutions that satisfy these boundary conditions for the algebraic equations defining the flow domain [1, 9].

The solver in the CFD code (FLUENT), is based on the finite volume methods, which integrates the governing equations in the finite volumes (control volumes) over the whole computational domain. There is one generic form of equation for one flow variable, ϕ which could be a velocity component, enthalpy or species concentration:

$$\frac{\partial \rho \phi}{\partial t} = -\nabla(\rho V \phi) + \nabla(\Gamma_{\phi} \nabla_{\phi}) + S_{\phi} \quad (1.1)$$

Where:

ϕ = dépendent variable

Γ_{ϕ} = exchange coefficient (laminar + turbulent)

V = flow velocity vector

ρ = flow density

S_{ϕ} = source of the variable

This integrated expression in equation (1.1) above means that the rate of change of ϕ in the control volume (cells from the mesh/grid) with respect to time is equal to the sum of the net flux of ϕ due to convection into the control volume, the net flux of ϕ due to diffusion into the control volume and the net generation rate of ϕ inside the control volume. Following integration, the solver uses various approximations, which are based on an application of the finite difference method, to replace all the terms in the integrated equation (the time-change rate, the convective and diffusive fluxes and the source term) [1].

This process converts the equation into a set of algebraic equations, which are ready to be solved by an iterative method. The iteration is the third and the last action the solver does in the whole computation task (simulation) [1].

1.2.3 Post-processor

The post-processor allows the CFD operator to construct a picture of the simulated flow problem by displaying the geometry of the problem, the computational domain and the mesh/grid system. It may then display contour or iso-surface plots for the flow variables, including contours plotted over specified surfaces, such as on a solid/fluid interface or an iso-surface of a second flow variable. In many cases velocity vector plotting is important, as is streamline presentation or particle tracking or pathlines [1].

A complete CFD simulation often requires repeating the procedure a number of times. It is not rare to run a large number of trials before reaching a set of reasonable solutions. The procedure includes tuning the mesh system, adjusting boundary conditions, selecting numerical parameters, finding the correct physical model, monitoring iteration and finally, viewing the results [1,13].

1.3 Hot-wire Chemical vapor deposition system

The technique of HWCVD is being increasingly used for the deposition of materials such as hydrogenated amorphous or microcrystalline silicon and its alloys and as diamond films. The main part of the deposition system consists in a vacuum chamber evacuated by a pumping unit to some appropriate vacuum level. After achieving the desired ultimate vacuum, the process of gas mixture is introduced via Mass flow controllers and the pressure is kept constant by a variable conductance valve. The process of gas is then decomposed by the heat generated by a hot filament of tungsten, tantalum or other material into radicals which are then deposited as thin films [32].

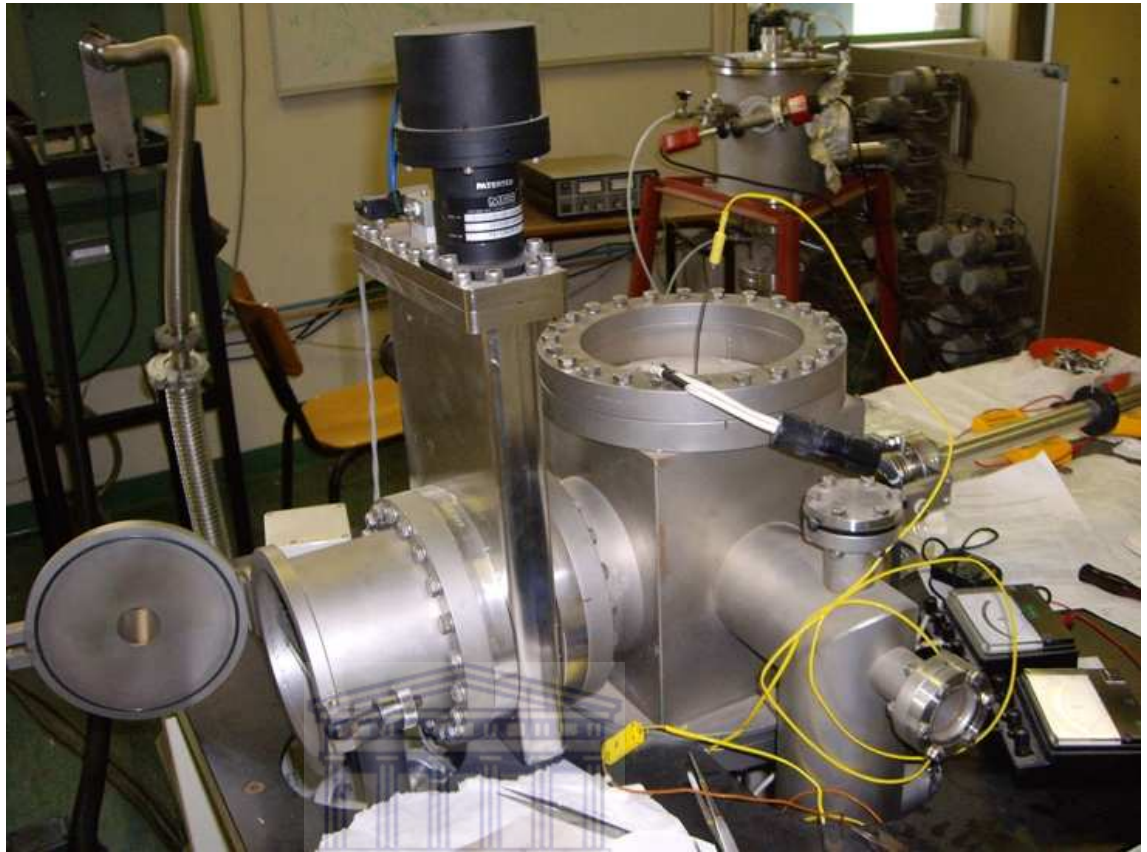


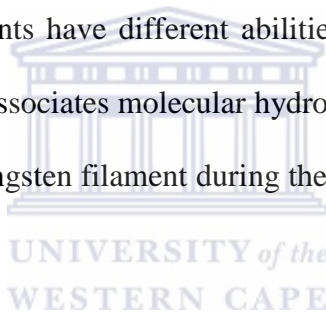
Figure1: The hot-wire chemical vapor deposition system used at the Physics department of the University of the Western Cape.

The HWCVD system, requires relatively simple apparatus, offer the advantages of high deposition rate, low hydrogen content and effective decomposition of gas molecules. HWCVD shows great potential in large area electronics application. For the application of this technique in commercial products, the uniformity of film thickness over a large scale is particularly important.

Usually, the thickness uniformity of film in HWCVD is mainly effected by gas supply, catalyzer structure, diffusion of radicals and the temperature distribution of

substrate. A uniform and sufficient gas flow is required, because the deposition process is a gas flow limited one [33].

The HWCVD process has been extensively used for the deposition of various materials, including diamond, polymers, silicon thin films, boron-carbon-nitride layers and carbon nanotubes. The process relies on the catalytic decomposition of precursor gases into reactive gaseous species by a resistively heated filament. A variety of transition metals, such as tungsten (W), tantalum (Ta) and rhenium (Re), have been utilized as the filament during the HWCVD process. This is primarily due to their high melting points and superior mechanical stabilities at temperatures above 1500°C. Furthermore, different filaments have different abilities to dissociate the precursors. For example, a Ta filament dissociates molecular hydrogen (H_2) into atomic hydrogen (H^0) twice as efficient as a tungsten filament during the deposition of microcrystalline silicon thin films [34].



1.4 *The Aim and Outline of this study*

In this study, we want to determine the mixture of the gas flow patterns inside the HWCVD system, by using the CFD software, FLUENT; using information known from the solar cells group of the physics department in the University of the Western Cape. This includes the flow rate of the silane gas (SiH_4) at 1.2 sccm (standard cubic centimeter) and for the hydrogen (H_2) gas at 58.8 sccm, which are the two gases used during the deposition on two substrates (silicon and glass). This information is then

used in this study to calculate the species mass fraction for the inlets boundary conditions.

The two gases (silane and hydrogen) are introduced into the HWCVD system with the two deposited substrates (silicon and glass) under a constant pressure of 60 μ bar and the heat flux of the filament is about $99.21 \times 10^3 \text{ W/m}^2$, by varying the temperature of the heater of 100 °C, 200 °C, 300 °C and 550 °C; the simulation shows how the temperature affects the flow of the gas flow patterns inside the system.

In the second chapter we will give an overview of the HWCVD; a short historical overview of the technique is given and key issues pertaining CFD and this study are discussed. We will look at the background of the finite volume method, the mathematics involved in CFD (the Navier-Stokes equations).

The third chapter will give a comprehensive simulation method for this study.

Chapter four will focus on the main results obtained from the simulation and discussions and conclusion. References are given at the end of the chapters in these study and appendices giving the description of the simulation method used in this study. The contour plots and pathlines showing the movement of the gas inside the CVD system obtained from the results in this study.

CHAPTER 2

TECHNIQUES USED IN THIS STUDY

2.1 HWCVD

2.1.1 Background

A HWCVD technique was introduced in 1979 by Wiesmann *et al* [7] as a method for producing hydrogenated amorphous silicon thin films. However, the results of Wiesmann were not encouraging because they used too low pressures of 5.33×10^{-4} mbar which resulted in a poor dark conductivity of the thin films as compared to the materials prepared by plasma enhanced chemical vapor deposition (PECVD). This technique has found its application in 1991 when Mahan *et al* reported on the development of device quality a-Si:H thin films with low hydrogen content [8].

The HWCVD technique is based on the deposition of the source gases, usually silane (SiH_4) or a mixture of H_2 and SiH_4 gases on a heated filament. This technique is also called the Catalytic Chemical Vapor Deposition (Cat-CVD). Figure 2.1 shows the schematic cross-section of the HWCVD reaction chamber; in this study the gas flow patterns inside the HWCVD are determined using a CFD software (FLUENT) as outlined in chapter 1. The source gases H_2 and SiH_4 are injected into the chamber and decomposed on a heated filament. On the way from the filament to the substrates (glass and silicon which are the two substrates), the constituent radical species

produced on the heated filament often react in the gas phase before deposition onto the heated substrate [8].

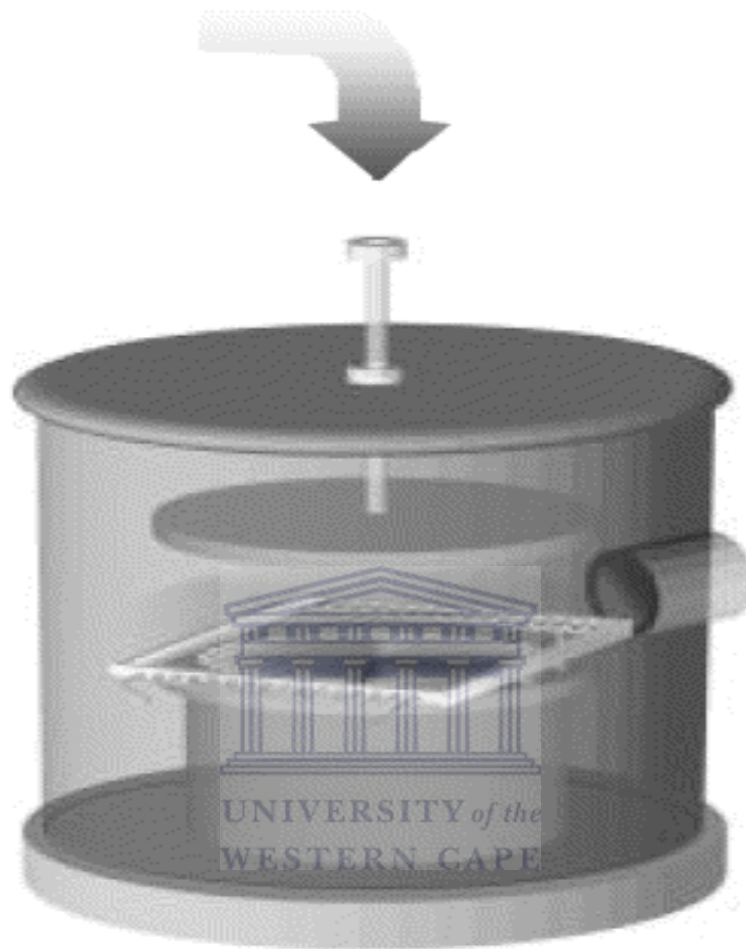


Figure 2.1: Schematic cross-section of an HWCVD system, with the inlet at the top and outlet on the side of the chamber [26].

Figure 2.1 above shows the cross-section of a HWCVD system. The deposition materials used in the HWCVD system in this study, by the solar cells group in the physics department of the University of the Western Cape, are based on H_2 and SiH_4 gases.

2.1.2 HWCVD Process

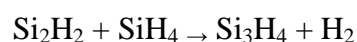
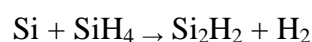
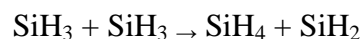
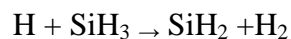
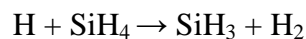
Hot-wire was first introduced by Wiesmann *et al.* [7] in 1979 when he succeeded to deposit a Si: H by thermal decomposition of silane from a hot tungsten or carbon foil heated to about 1600°C. Unfortunately due to very low gas pressures (1.33×10^{-6} – 1.33×10^{-4} mbar), he achieved too low deposition rates (0.6 – 8.7 Å/sec) and films with low quality due to the surface filament were not understood at that stage. Evidence of the catalytic nature of the decomposition has now been found: The 12.9 eV needed to pyrolytically cleave four Si-H bonds [27] is much higher than the activation energy of Si radical on the surface of the main wires used (Mo, Ta and W) of (2.6, 1.0, and 0.74 eV) respectively as reported by Tange *et al* [28].

Later, in 1986 Matsumura [29] obtained high quality hydro-fluorinated a-Si (a-Si: F: H) and hydrogenated amorphous silicon (a-Si: H) by thermal catalytic reactions between deposition-gas and a heated tungsten catalyzer. He named it “catalytic – CVD (CTL- CVD)” method. A deposition rate larger than 20 Å/sec was achieved and more importantly, he reported that the magnitude of the SWE of the films produced seemed smaller than that of the glow discharge a-Si: H produced films.

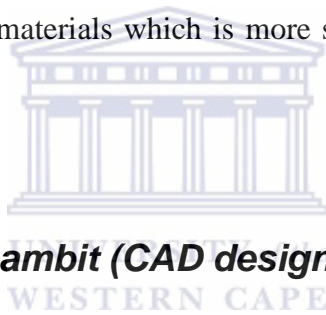
J. Doyle *at al* [30] using what they referred to an “evaporative surface decomposition (ESD) method” reported in 1988 a deposition of excellent a-Si: H film quality from silane decomposition with silane pressures ranging from 4 to 30 mTorr (-5 – 40 μbar). They explained the deposition mechanism and postulate for the first time the nature of the radicals giving growth at the substrate surface. As actually agreed upon, they identified the 3 main phases of the deposition process:

1. The deposition of the feed gas on the hot surface of the wire.
2. The evaporation of the radicals and gas-phase collision (creation of secondary species).
3. Film growth on the substrate surface.

At the -1700 K filament temperature where they were working, they noted that the decomposed silane gas was mostly atomized into H and Si atoms. A major fraction of the Si and H atoms is expected to arrive at the substrate without reacting, but a significant fraction may react to form other radicals. Hot Hydrogen and silicon atoms which have not undergone the gas-phase collisions process were observed to dominate the radical flux to the hydrogen-passivated a-Si: H surface. They observed that the dominant species impinging on the substrate were SiH₄ and H₂. The reaction between SiH₄ and the surface dangling bond was postulated to give SH₃ and a passivated surface bond. Thus considerable Si H₃, lesser SiH₂ and Si₂H₂ (which increase with the gas pressure) were expected to contribute to the deposition. J. Perrin *et al* [31] have confirmed the nature of these radicals as exothermic gas phase reactions in the HWCVD:



In 1991, Mahan *et al* [8] demonstrated for the first time the possibility to produce device-quality a-Si: H with reduced hydrogen content. Good quality films with less than 1 at. % hydrogen compared to 8-12 at. % contained in good quality a-Si: H obtained by plasma enhanced CVD, confirmed that only a small quantity of hydrogen was needed to passivate the dangling bonds. Mahan and co-authors obtained thin films with photosensitivity (σ_p/σ_d) – 10^5 and Urbach edges that, in contrast to PECVD films, did not broaden as the hydrogen content was reduced. After the work of Mahan, many groups worldwide took a keen interest in this Si-based new technology. Efforts have been focused on the understanding of the deposition process itself, the issues related to the growth and improvement of the deposition rate on the deposition of a new class of materials which is more stable and less sensitive to the SWE [15].



2.2 Background on Gambit (CAD design)

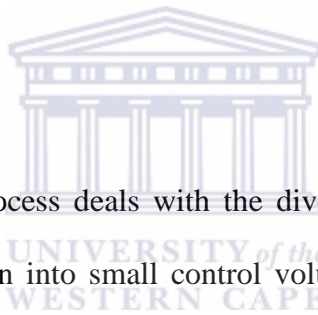
Gambit was released on summer 2004; its focus was to be on CAD import, geometry conditioning and automatic meshing. This is the first step in building and analyzing a flow model. It includes building the model within a CAD package, creating and applying a suitable computational mesh/grid, and entering the flow boundary conditions and fluid materials properties. These pre-processor tools used in this study, called Gambit is part the packaged software FLUENT [1, 9].

CAD geometries are easily imported and adapted for CFD solutions in Gambit, which is FLUENT's own pre-processor step. The three dimensions (3D) solid modeling option in Gambit allows for straightforward geometry constructions as well as high

geometry translation. This means that the geometry can be translated in three dimensions. Among a wide range of geometry tools, Boolean operators provide a simple way of getting from a CAD solid to a fluid domain [9].

A state-of-the-art set of cleanup and conditioning tools prepares the model for meshing. Gambit's unique curvature and proximity based "size function" produces a correct and smooth CFD-type mesh throughout the model. Together with a boundary layer technology, a number of volumetric meshing schemes produce the correct mesh for your application. Parametric variations are also inherent to the process [1, 9].

2.3 Mesh Generation



The mesh/grid generation process deals with the division of the domain (designed geometry) under consideration into small control volumes on which the discretised governing equations will be solved. The grid generation forms a large part in terms of person-hour time of the CFD analysis. Gambit, is the CAD design system used in this study to design a domain/geometry and generate a grid/mesh from the designed domain [9,14].

Gambit uses solid modeling techniques to create a virtual model of the geometry under consideration. There are various grid generation tools available to create a grid/mesh in this geometry. The grid/mesh generation tools are available to create hexahedron, tetrahedron, prism and pyramid cells [9].

The origin of the term mesh/grid goes back to early days of CFD when most analyses were 2D in nature. For 2D analysis, a domain split into elements resembles a wire mesh, hence the name. These process of obtaining an appropriate mesh/grid is termed mesh generation (or grid generation) [9,14].

Below there are pictures of the designed domain/geometry and its mesh/grid using the CAD design system, Gambit.

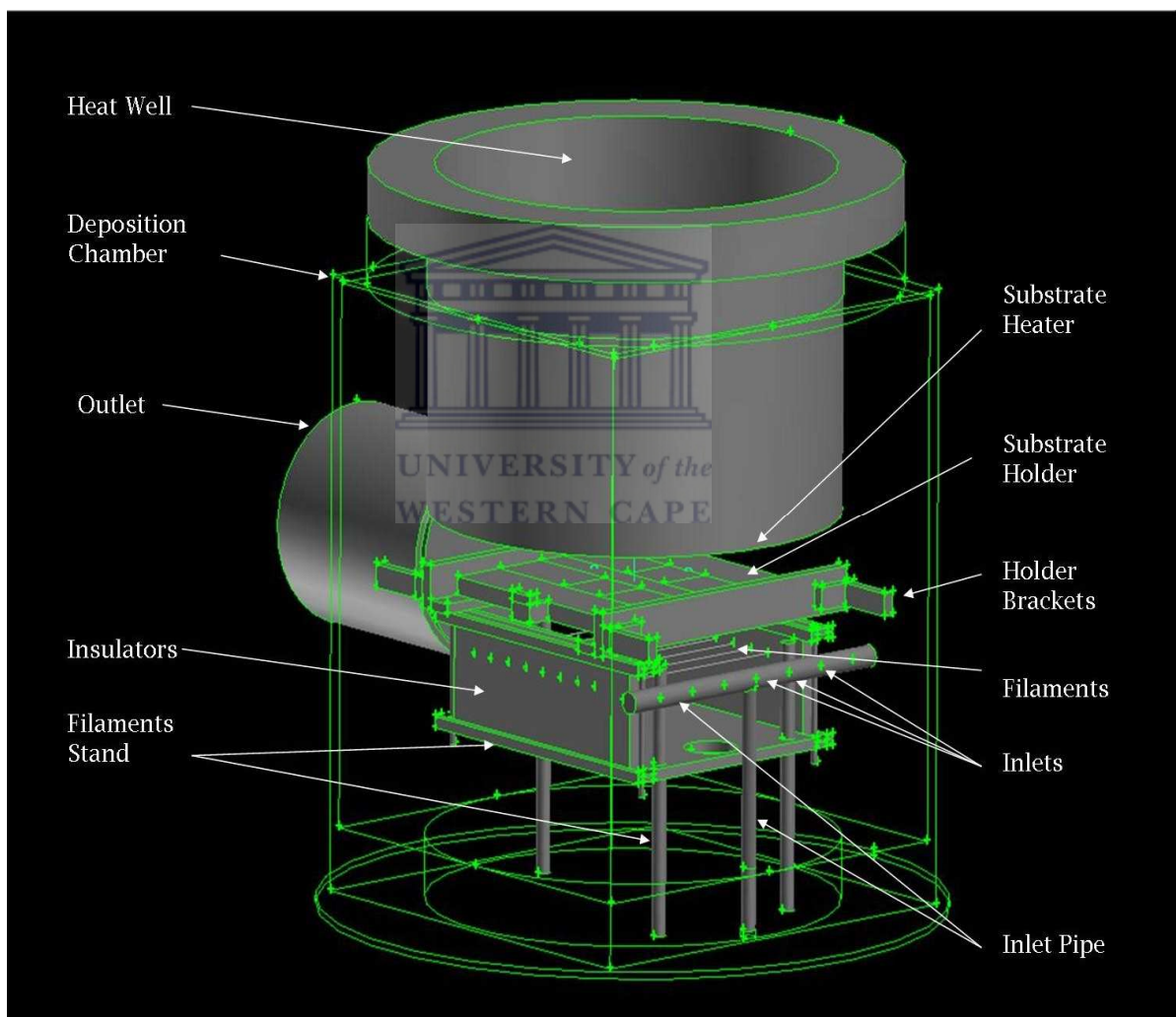


Figure 2.2: A domain (geometry) of the HWCVD system as used in this study, designed using the CAD design system GAMBIT.

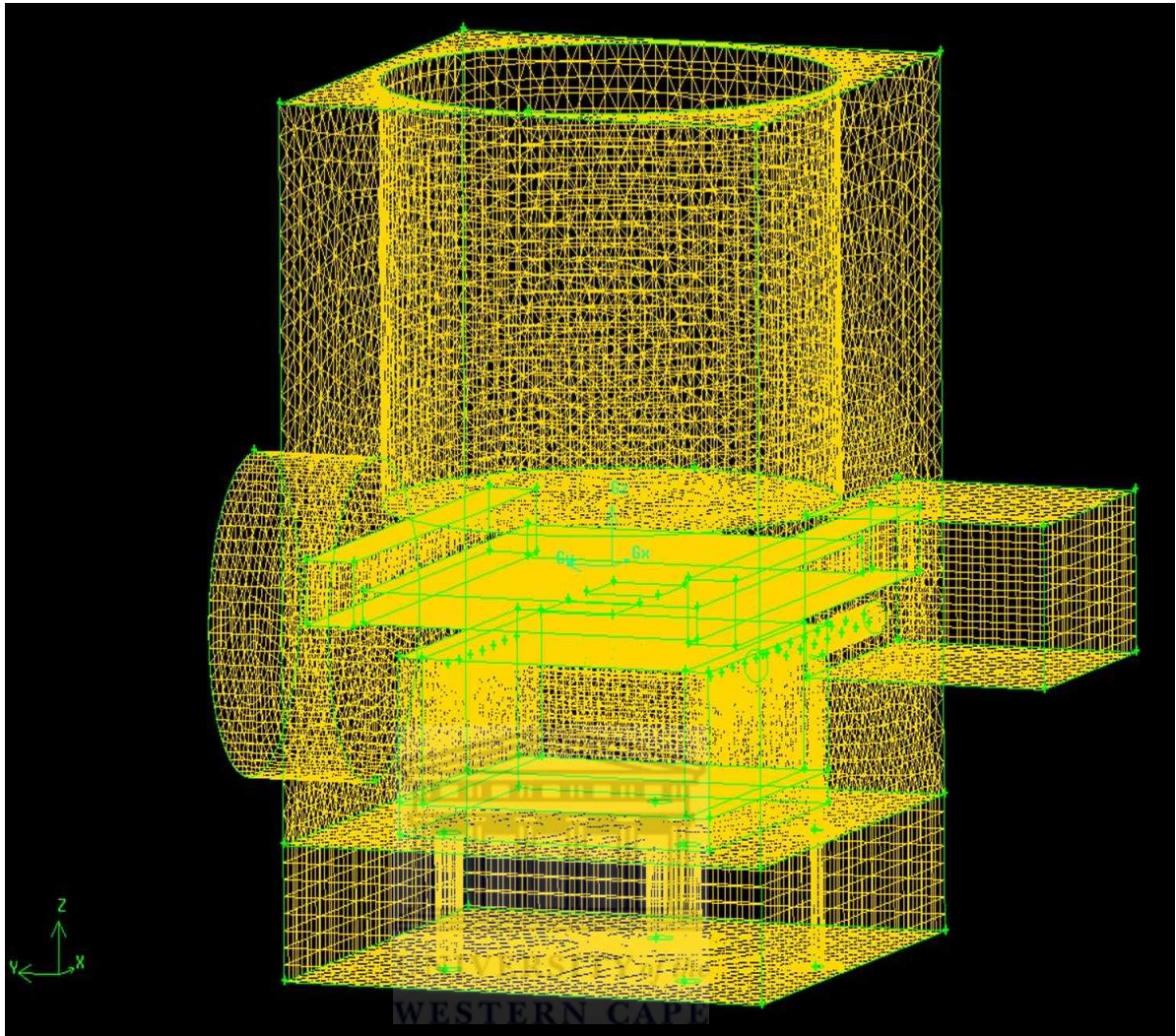


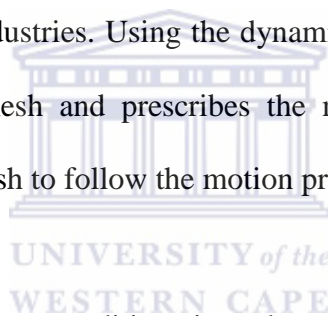
Figure 2.3: A grid (a mesh) of the HWCVD system as used in this study, designed using the CAD design system GAMBIT.

2.4 Background on FLUENT

FLUENT is the computer software package of CFD which was used in this study to model the gas flow patterns inside the HWCVD system. Fluent is the general name for the collection of computational fluid dynamics programs sold by Fluent Inc. of Lebanon, New Hampshire, USA [11].

As outlined in chapter one, every CFD code consists of three basic components, the pre-processor (CAD design; Gambit), the solver which is the heart of the CFD code carrying out the major computations and providing the numerical solutions, and the post-processor for constructing pictures of plots of the simulated problem. The FLUENT software package which was used in this study is the FLUENT version 6.3.26, where the geometry was designed and meshed in Gambit saved and then exported the mesh to FLUENT for running the simulation.

Fluent is a general-purpose CFD code based on the finite volume method on a proper order grid/mesh. Fluent technology offers a wide array of physical models that can be applied to a wide array of industries. Using the dynamic and moving mesh: The user simply sets up the initial mesh and prescribes the motion, while fluent software automatically changes the mesh to follow the motion prescribed [11].



This is useful for modeling flow conditions in and around moving objects. There are many spectral methods available in CFD, but in this study the one that will be used is the Finite Volume Method [11]. The numerical solution method used in FLUENT (Finite Volume Method), will be discussed below.

2.5 Finite Volume Methods

The finite volume method is a method for representing and evaluating partial differential equations as algebraic equations. This is similar to the finite difference method, where values are calculated at discrete places on a meshed geometry [11,20].

The phrase ‘finite volume’ refers to the small volume surrounding each node point on a mesh. In this method, volume integrals in partial differential equations that contain a divergence term are converted to surface integrals, using the divergence theorem. These terms are then evaluated as fluxes at the surfaces of each finite volume. Because the flux entering a given volume is identical to that leaving the adjacent volume, these methods are conservative [11,23].

Another advantage of the finite volume method is that it is easily formulated to allow for unstructured meshes. As mentioned above, this method is used in the computational fluid dynamics package; Fluent [11].

2.6 Mathematics behind CFD



The fundamental basis of any CFD problem is the Navier-Stokes equations, which define a single phase flow. The most fundamental consideration in CFD is how one treats a continuous fluid in a discretized fashion on a computer. One method is to discretize the spatial domain into small cells to form a volume mesh/grid, and then apply a suitable algorithm to solve the equations of motion [4,5]. Below we will discuss the conservation equations which describe the flow field.

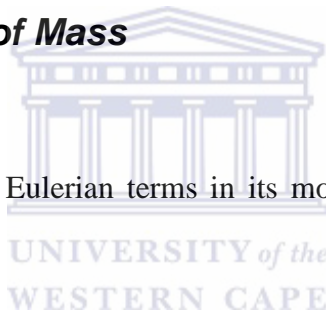
2.6.1 Navier-Stokes Equations

The governing equations that describe the flow field are a set of non-linear partial differential equations. The equations are derived from mass, momentum and energy

conservation. In chapter 1 it was outlined that the Navier-Stokes equations are a complex non-linear set of partial differential equations that describes the mass, momentum conservation of fluid.

In the past, engineers made further approximations and simplifications to the equation set until they had a group of equations that they could solve. Recently, high speed computers have been used to solve approximations to the equations using a variety of techniques like finite difference, finite volume, finite element, and spectral methods which are in the area of CFD [4,5,24].

2.6.1.1 Conservation of Mass



The conservation of mass in Eulerian terms in its most common form for fluids is given as follows:

$$\frac{\partial \rho}{\partial t} + \text{div} \rho V = S_m \quad 2.1$$

Where ρ is the density, t is the time, V is the velocity vector of the fluid and S_m is a mass source. For a constant density, equation 2.1 will reduce to the following:

$$\text{div} V = 0 \quad 2.2$$

2.6.1.2 Momentum equations

The Navier-Stokes equations are derived from the conservation of momentum (Newton's second law). The set of equations can be written in Eulerian terms as single vector equations using the indicial notation:

$$\rho \frac{DV}{Dt} = \rho g - \nabla p + \frac{\partial}{\partial x_j} \left[\mu \left(\frac{\partial v_i}{\partial x_j} + \frac{\partial v_j}{\partial x_i} \right) + \delta_{ij} \lambda \text{div} V \right] \quad 2.3$$

Where g is the gravitation vector, x_i is the spatial co-ordinate, v_i is the i -component of the velocity vector, μ is the ordinary coefficient of viscosity, λ is the coefficient of bulk viscosity, δ_{ij} is the Kronecker delta function ($\delta_{ij} = 1$ if $i = j$ and $\delta_{ij} = 0$ if $i \neq j$) and $\frac{D}{Dt}$ is the total or substantial derivative. The relation between the ordinary viscosity and bulk viscosity is given by the Stoke's hypothesis [18]:

$$\lambda + \frac{2}{3} \mu = 0 \quad 2.4$$

An example of the equations 2.3 in the i -direction is written as follows:

$$\rho \frac{Du}{Dt} = \rho g_x - \frac{\partial p}{\partial x} + \frac{\partial}{\partial x} \left(2\mu \frac{\partial u}{\partial x} + \lambda \text{div} V \right) + \frac{\partial}{\partial y} \left[\mu \left(\frac{\partial u}{\partial y} + \frac{\partial v}{\partial x} \right) \right] + \frac{\partial}{\partial z} \left[\mu \left(\frac{\partial u}{\partial z} + \frac{\partial w}{\partial x} \right) \right] \quad 2.5$$

2.6.1.3 Energy equations

The energy equation is derived from the first law of thermodynamics. The energy relation in Eulerian terms is given by the following if it is assumed that the conduction heat fluxes are given by Fourier's law and that radiative effects are negligible [4,24]:

$$\rho \frac{Dh}{Dt} = \frac{Dp}{Dt} + \text{div}(k\nabla T) + \Phi \quad 2.6$$

Where h is the fluid enthalpy, k is the thermal conductivity, T is the temperature of the fluid and Φ is the viscous dissipation and is given as follows:

$$\Phi = \mu \left[2\left(\frac{\partial u}{\partial x}\right)^2 + 2\left(\frac{\partial v}{\partial y}\right)^2 + 2\left(\frac{\partial w}{\partial z}\right)^2 + \left(\frac{\partial v}{\partial x} + \frac{\partial u}{\partial y}\right)^2 + \left(\frac{\partial w}{\partial y} + \frac{\partial v}{\partial z}\right)^2 + \left(\frac{\partial u}{\partial z} + \frac{\partial w}{\partial x}\right)^2 \right] + \lambda \left(\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} + \frac{\partial w}{\partial z}\right)^2 \quad 2.7$$

If assuming incompressible flow as well as constant thermal conductivity and low-velocity flow where the viscous dissipation (Φ) is zero, the equation 2.7 above will reduce to the following equation:

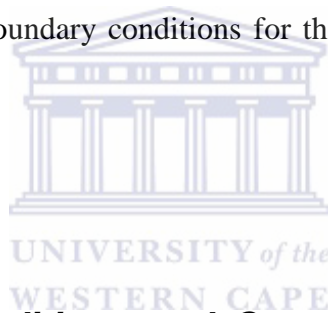
$$\rho c_p \frac{DT}{Dt} = k\nabla^2 T \quad 2.8$$

The equations under 2.5.1.1 to 2.5.1.3 are the equations which are used in every CFD simulation; as mentioned under 2.5 that the fundamental basis of any CFD problem is

the Navier-Stokes equations which are non-linear partial differential equations; derived from mass, momentum and energy conservation.

In this study, these equations are used by the computer by default under the solver stage to determine the mixture of the gas-flow patterns inside the HWCVD system; derived from mass, momentum and energy conservation.

The solver as outlined in chapter 1 has two components in solving the computational simulation. One of these components is to convert the partial differential equations and the boundary conditions formulae into a group of algebraic equations and then, the second component of the solver stage is to use the iterative procedure to find solutions that satisfy these boundary conditions for the algebraic equations defining the flow domain.



2.7 Steady State conditions and Computational accuracy in

FLUENT

A steady state calculation yields a solution in a shorter execution time in comparison to a transient calculation. Nonetheless, there may be some underlying circumstances, where convergence and/or stability cannot be guaranteed through the steady state approach and a transient calculation may be required to march the numerical procedure toward the steady-state condition. Other issues concerning the aspects of computational accuracy and efficiency can also have a strong influence of the CFD solution. Subject to the availability of computational resources, it is nearly always inevitable that some compromise has to be reached for solving complex CFD problems.

By increasing the number of cells (i.e. with decreasing the mesh spacing) in the computational domain geometry, the accuracy of the computational solution is usually enhanced. There is, however, a trade off that needs to be considered between increasing computer storage running-time. One possible way that comparable accuracies can be obtained on a courser mesh while maintaining computational efficiency is to employ higher order discretization schemes to solve such problems.



CHAPTER 3

SIMULATION METHODS

3.1 Simulation Methods

In this section the simulation procedure that was followed in determining the mixture of the gas flow patterns inside the HWCVD system using the Fluent software package, will be outlined. From the previous chapter (chapter 2), a detailed background of the software package was given with the different tools that it is comprised with.

The software package has a Cad design system (GAMBIT), in which the geometry of the system to be modeled is generated and meshed using the tools in the Cad design system. The Cad system also enables the user to set (define) the boundary conditions for the different part of the system, which will again be set in the second stage of the software; the solver stage. This stage of the software is known as the heart of the software package, because this is where most of the simulation work is being done. Under this stage, the user input the parameters to be considered in the simulation process, the boundary conditions are also set under this stage; selecting from the tools that are there in the package the materials to be used inside the system designed using the Cad design system.

In this study, the materials that were selected to be used under the solver stage are the two gases (H_2 and SiH_4) and the two substrates that are deposited inside the HWCVD system (glass and silicon). The properties of silicon and glass (i.e. the thicknesses, thermal conductivities, the pressure inside the HWCVD system) are also defined under the solver stage. The calculation (simulation) of determining the

mixture of the gas flow patterns inside the HWCVD is done by the computer using the process of iteration in the Fluent software package. The flow chart below is a step by step illustration of the simulation procedure followed in any CFD simulation problem.

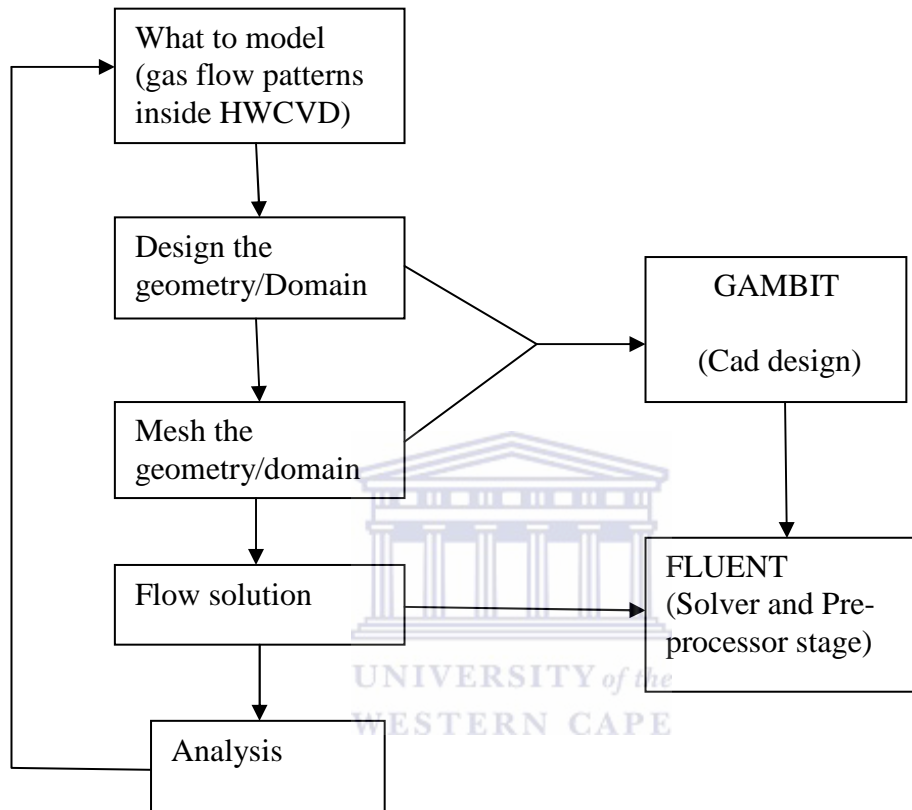


Figure 3.1: A flow chart of the procedure followed in a CFD problem (simulation).

3.2 Designing the Domain/Geometry

The first step of any simulation problem is to decide on what to model; which in this study is to model the mixture of the gas flow patterns inside the HWCVD system using the CFD software package FLUENT. As it was outlined in chapter 1, the pre-processor stage of the Fluent software is comprised with a Cad design (GAMBIT) system to create the geometry of the system to be modeled. In designing the HWCVD

chamber in the Cad design system, the dimensions of HWCVD system was collected by measuring the different parts of the system. The table below shows the collected data for the dimensions of the HWCVD system to be used to design its domain/geometry by using the Cad design system.

Table 3.1 Some of the measurements of the HWCVD system.

Name of the part	Height (length) measurement in mm	Diameter measurements in mm
Gas inlet tube	130	9.7
Outlet	50	179
Insulators	44	9.7
Filaments	11	0.1
Filaments-stand	5	121.5
HWCVD system	300	Rectangular shape
Glass (substrate)	0.8	Rectangular shape
Silicon (substrate)	0.4	Rectangular shape
Substrates-holder	122	Rectangular shape
Heater	128	Rectangular shape

The table above has only the parts of the geometry which were used in this study; some parts of the geometry which were measured were not used due to the small influence that they will have to the gas flow and they were increasing the number of cells in the grid/mesh thus increasing the computing time of the simulation.

Having the measurements of the internal and external geometry of the HWCVD; the geometry of each part was designed individually using the CAD design program

(Gambit) and combined to the exact space inside the system (HWCVD) for determining the gas flow.

As outlined in chapter 2; Gambit offers many options in designing the geometry, each of these parts were designed to its specific size and shape; by scaling them to fit in the computer using Gambit. Figures 3.2 and 3.3 below, shows the parts of the chamber which were designed individual, each with its own measurements; and then in figure 3.4 there is a domain of the chamber with all the parts included inside it.

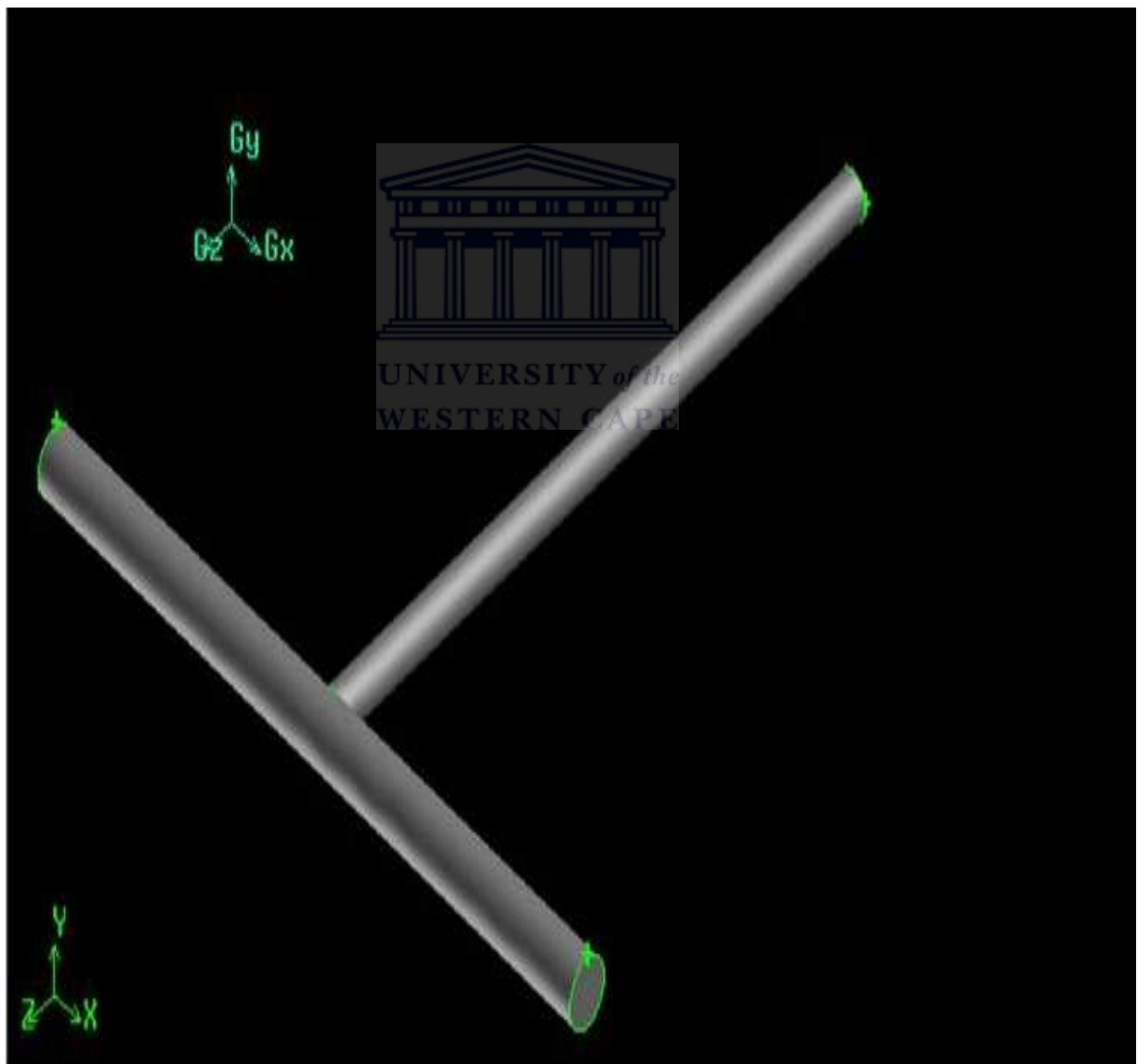


Figure 3.2: a domain of gas-inlet pipes.

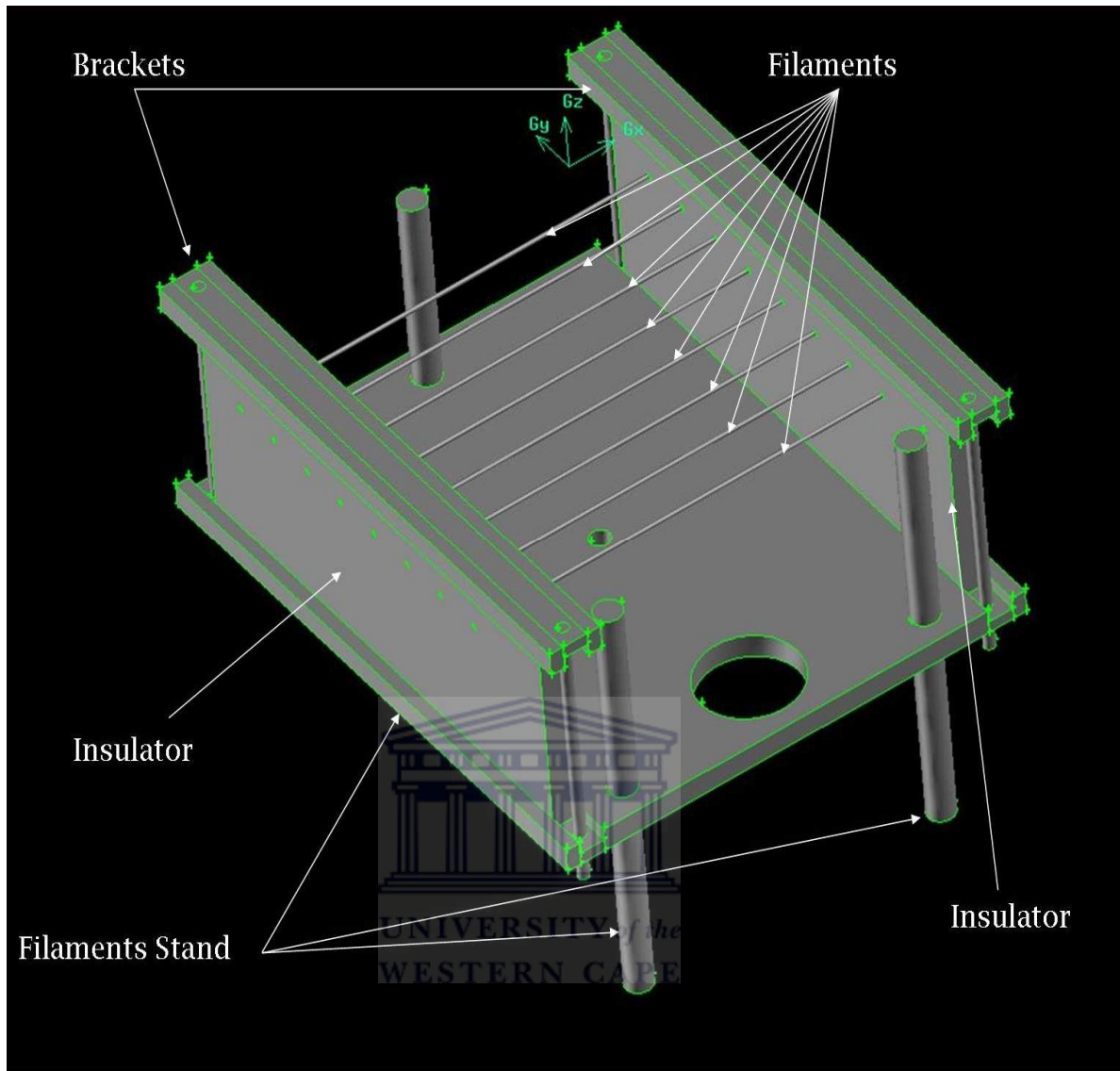


Figure 3.3: a domain of the filaments, insulators and filaments stand.

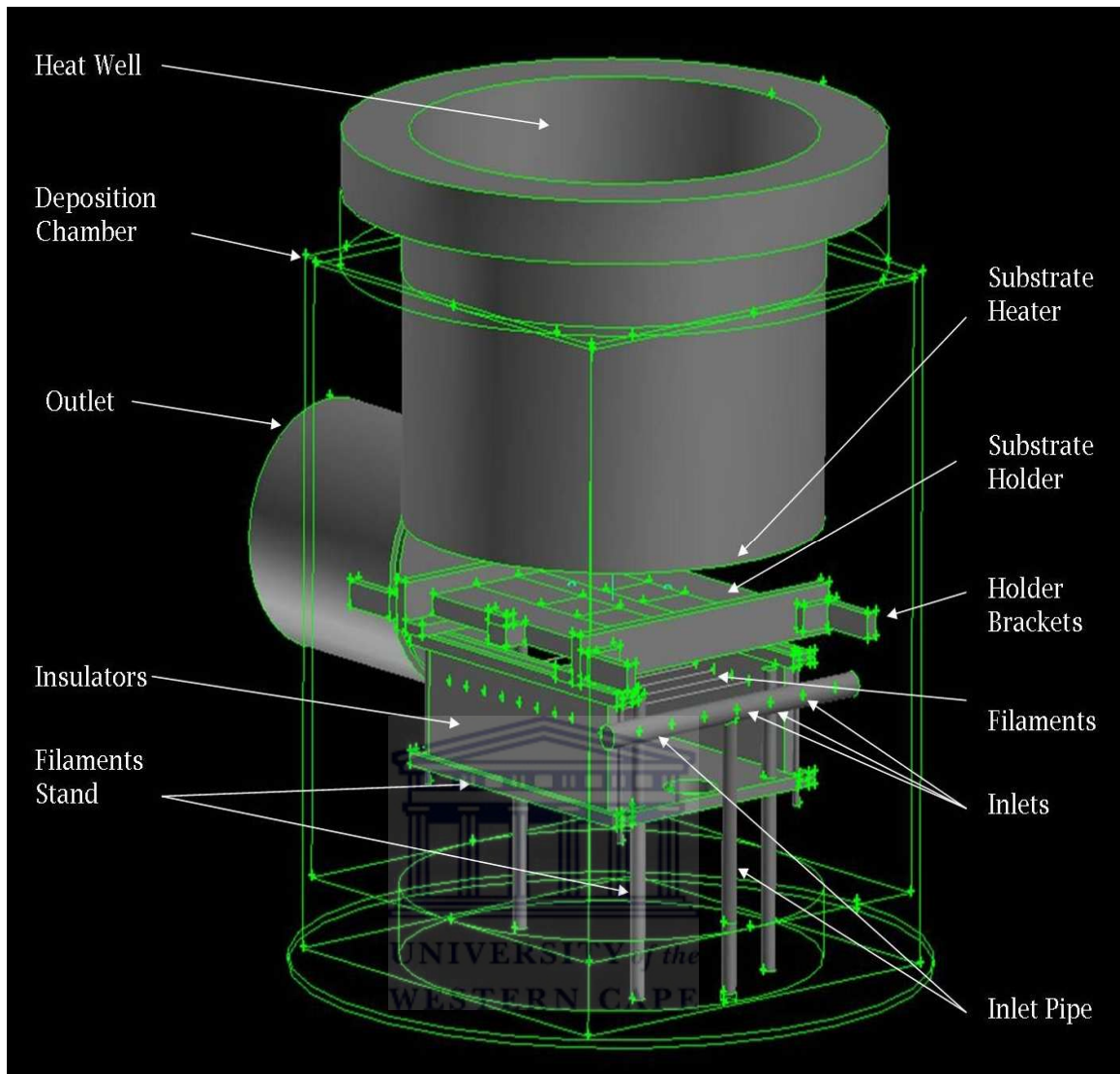


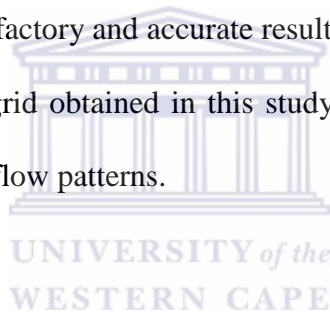
Figure 3.4: Deposition chamber (CVD) with all the parts imported to it by Gambit.

All the parts were designed individually and each of them saved in Gambit as xx.dbs files (the format used in the Gambit CAD design system for storing files). These parts were then imported to the chamber by using the measurements obtained at the beginning of the study in placing them in their correct positions inside the chamber in order to get the completed HWCVD chamber as given above in figure 3.4.

In every CFD simulation process the designed geometry of the system to be modeled has to be meshed in order to have a complete designed system to start the simulation process. This process of meshing was done in this study after having the geometry given in figure 3.4. As mentioned in chapter 2, there are a number of tools which are offered by Gambit in generating the mesh, one of the tools which was used in this study to obtain a finer mesh; is the size functioning tool.

The mesh obtained in any CFD problem, affects directly the accuracy of the solution and the cost of computation, in terms of computation time and hardware requirement. An optimized mesh/grid system uses less computer memory space, requires less computing and yet gives satisfactory and accurate results [1,2,9].

Figure 3.5 below is a mesh/grid obtained in this study for the HWCVD chamber to model the mixture of the gas flow patterns.



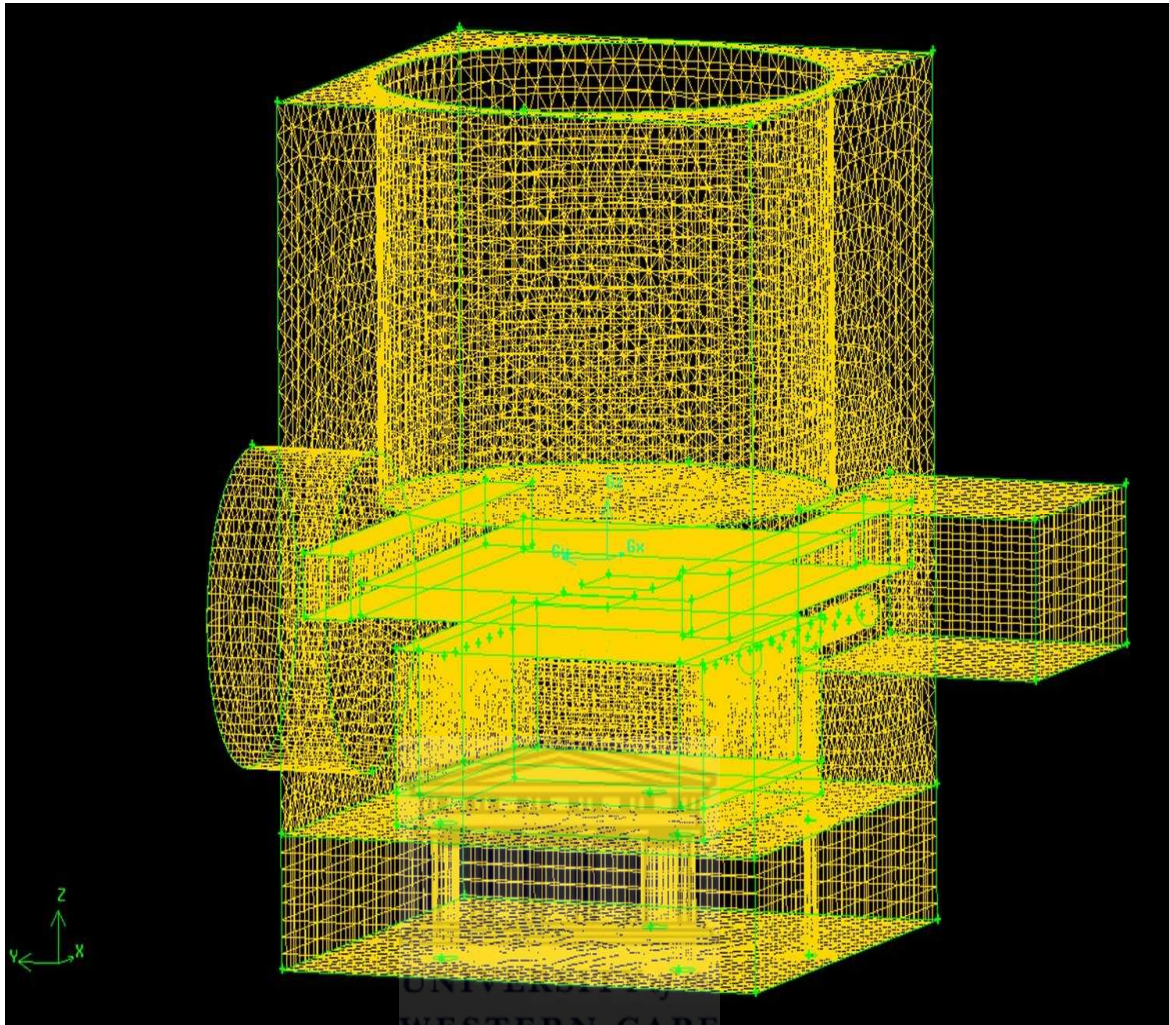


Figure 3.5: a grid (a mesh) of CVD system, with the total number of 657120 cells.

3.3 The deposition parameters of the HWCVD system

The HWCVD system is used by the solar energy research facility at the University of the Western Cape. The process of the HWCVD system, involves the deposition of the two substrates by using the H_2 and SiH_4 gases under a constant pressure of $60\mu\text{bar}$ by varying the temperature of the heater, these process will be performed in this study using the CFD software package; FLUENT. The table below is the general data of the HWCVD system with the four varying temperatures of the heater which will be used

in the simulations of this study to determine the gas flow patterns inside the deposition system.

Table 3.2: The deposition parameters used in the HWCVD system.

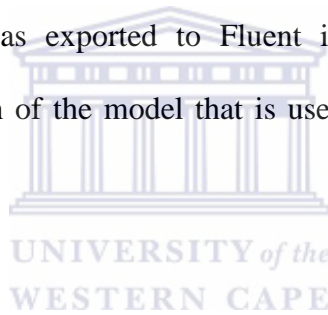
Pressure of HWCVD	60 μ bar
Temperature of the Heater	100 °C, 200 °C, 300 °C and 550 °C
Temperature of the filaments	1600 °C
Heat Flux around the filaments ^(Appendix A.3)	$99.21 \times 10^3 \text{ Wm}^{-2}$
H ₂ mass flow rate	58.8 sccm
SiH ₄ mass flow rate	1.2 sccm

This data in the above table, it is some of the parameters used in the solver stage of the software before starting the simulation (iteration process). The heat flux of the filament is calculated using its temperature of 1600°C, this calculation is given in appendix A as well as the calculations for the mass flow rate of H₂ and SiH₄. After obtaining the mesh/grid given in figure 3.7, the boundary conditions for the walls (parts of the system) which were formed during mesh/rid generation where set in the Cad design system. Below is a table of the boundary conditions specified in the Cad design system (Gambit) in this study.

Table 3.3: Boundary conditions of the parts of HWCVD system.

Name of the Parts	Boundary Conditions
Inlets	Velocity-inlet
Outlet	Pressure-outlet
Wall (Chamber)	Wall

All the other parts inside the HWCVD (the two substrates (glass and silicon), substrates-holder, filaments, insulators, and heater) which are not given in Table 3.3 were specified as wall boundary condition. After completing the process in the Cad design system, the mesh was exported to Fluent in order to start running the simulation. A full description of the model that is used in this study is given in the appendix A.



The CFD software package (FLUENT) uses the Navier-Stokes equations and energy balances over control volumes, small volumes within the geometry at a defined location representing the HWCVD internals. The size and number of control volumes (mesh density) is user determined and will influence the accuracy of the solution to a degree. After boundary conditions have been introduced in the system (this is done automatically in Gambit when generating a mesh/grid), the flow and energy balances are solved numerically.

3.4 Starting the Simulation in FLUENT

The process of starting the simulation is done under the second stage of the Fluent software, the solver stage. The file which was created in Gambit and exported to

Fluent, will be opened in this stage in order continue with the simulation problem. The boundary conditions are being set the same as the boundary conditions which were set in the Cad design system and setting up the parameters inside the system. The material properties which are used in determining the mixture of the gas flow patterns are also defined under this stage. The HWCVD system has a number of parts with different material properties. The material properties for the HWCVD system used in this study are given in the table below.

Table 3.4: Material properties used in this study.

Material Properties	Specific Heat (C_p) (J/kg/K)	Density (ρ) (kg/m³)	Thermal conductivity (K) (W/m/K)
<i>Glass</i>	700	2579	1.05
<i>Alumina (Al₂O₃)</i>	880	961	18
<i>Tantalum (Ta)</i>	140	16690	57.5
<i>Silicon (Si)</i>	700	2329	130
<i>Copper (Cu)</i>	381	8978	387.6
<i>Steel</i>	502.48	8030	16.27

From the table given above of the material properties, glass and silicon are the two substrates used in the deposition process with thicknesses 0.08 cm and 0.04 cm respectively; Alumina (Al₂O₃) is the material used for the two insulators of the chamber, Tantalum (Ta) is the material for the filaments of the chamber, Copper (Cu) is the material of the inlets-pipe of the CVD chamber and Steel is the material used for the substrates-holder, heater, filaments-stand and Wall (chamber).

In this study, the segregated solution method of FLUENT was used. In this approach, the governing equations are solved sequentially (i.e. segregated from one another). Because the governing equations are non-linear (and coupled), several iterations of the solution loop must be performed before a convergence is obtained. Each iteration process consists of the steps illustrated in the figure [3.8] and outlined below [9,15]:

- Fluid properties are updated based on the current solution (if the calculation has just begun the fluid properties will be updated based on the initialized solution).
- The u, v and w momentum equations are each solved in turn using current values for pressure and face mass fluxes, in order to update the velocity field.
- Since the velocities obtained in the previous step may not satisfy the continuity equation locally, a “Poisson-type” equation for the pressure correction is derived from the continuity equation and the linearised momentum equations. This pressure correction equation is then solved to obtain the necessary corrections to the pressure and velocity fields and face mass fluxes such that continuity is satisfied [15].
- Equations for scalars such as energy and species are solved using the previously updated values of the other variables.
- When all these steps are met in a simulation, then a check for convergence of the equation set is made [15].

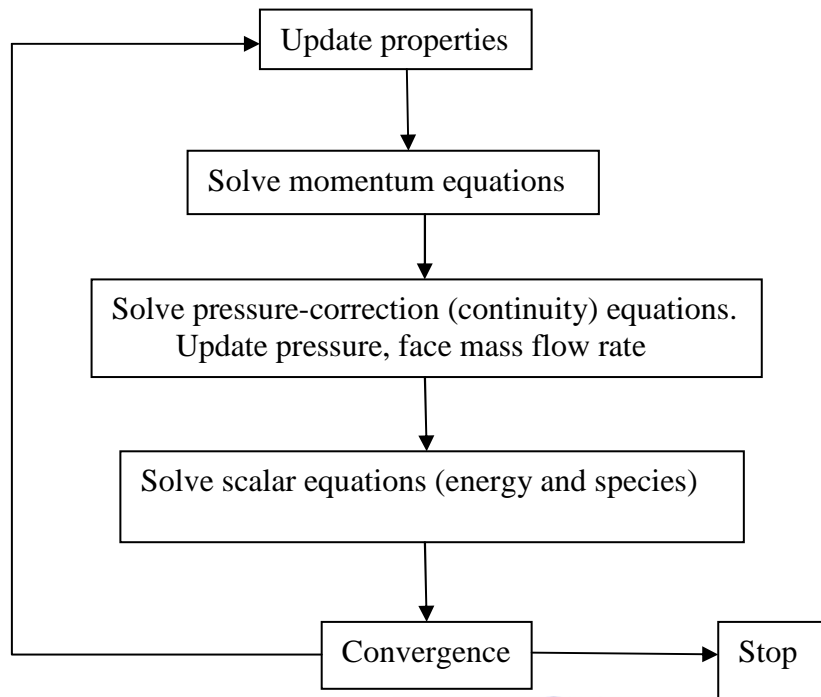


Figure 3.6: An overview of the segregated solution method when iterating [15].

An iterative process decreases the error in the solution until a satisfactory solution has been reached (i.e. the simulation is converged). The iterative process is the final step of the solver stage which is the process used to start the simulation. Each simulation in this study was calculated for 10000 iterations. The total number of simulations performed in this study is about four simulations; each simulation was performed using the same procedure outlined above, but with a different temperature of the heater (i.e. 100 °C, 200 °C, 300 °C and 550 °C). The results obtained from the four simulations after all this procedure is done (when the simulation is converged) will be given and discussed in the next chapter.

CHAPTER 4:

RESULTS AND DISCUSSIONS

4.1 Introduction

This section focuses on the results obtained in determining the gas flow patterns inside the hot-wire CVD system. There are a number of simulations which were performed in this study for one to come into having these results. As mentioned in chapter one under post-processor, a complete simulation often requires repeating the procedure a number of times. This includes tuning the mesh system, adjusting boundary conditions, selecting numerical parameters, finding the right physical model, monitoring the iteration and viewing the results.

The results in this chapter are for the simulations which were done under constant pressure of 60 μbar , constant heat flux of the filaments of the HWCVD of about $99.21 \times 10^3 \text{ Wm}^{-2}$ (Appendix A.3); by varying the temperature of the heater from 100 °C, 200 °C, 300 °C and 550 °C, thus the simulations show how the temperature affects the gas-flow patterns inside the HWCVD system. The results will give an indication of what influence the mass flow-rate and the surface deposition-rate of the mixture of gas particles inside the HWCVD system.

The results for the four simulations performed will be given and discussed in this chapter. There are two parts of the results which we will concentrate on in this study, that is, the results for the mass flow rate of the gas around the following important parts of the system; the filaments, the two substrates, inlet and outlet of the HWCVD

system. The second part of the results is the results for the surface deposition rate around the filaments, the two substrates and the substrates-holder inside the HWCVD system.

4.2 Mass flow-rate

This part of this study is about the mass flow-rate results. Table 4.1 is the results for the mass flow-rate obtained from the four simulations performed in this study, followed by the plot (graph of the mass flow-rate around the filaments, the two substrates, the inlet and outlet versus the temperature of the heater). The results in this table (table 4.1) show the values for the mass flow-rate into the system from the first to the fourth column of the results to be positive. The positive value means the mass flow-rate into the system through the inlets, and the negative mass flow-rate values indicates the total mass flow-rate out of the system through the outlet.

The results in table 4.1 also shows that the mass flow-rate out of the system is greater than the mass flow-rate flowing into the system, this is because of the small value of the velocity magnitude for the inlets which was calculated in chapter 3 to be $0.18^{(A.2)}$ using the flow-rate of the two gases ($H_2 = 58.8 \text{ sccm}$ and $SiH_4 = 1.2 \text{ sccm}$) flowing into the HWCVD system. Thus this value (velocity magnitude) makes the constants value of the flow into the system through the inlet to be small (5.74×10^{-12}).

In table 4.2 below, are the results for the surface deposition-rate obtained from the four simulations performed in this study, followed by a graph of the surface

deposition-rate (around the filaments, the two substrates and the substrates-holder) versus the temperature of the heater for all simulations.

Table 4.1 Mass flow-rate results for all simulations.

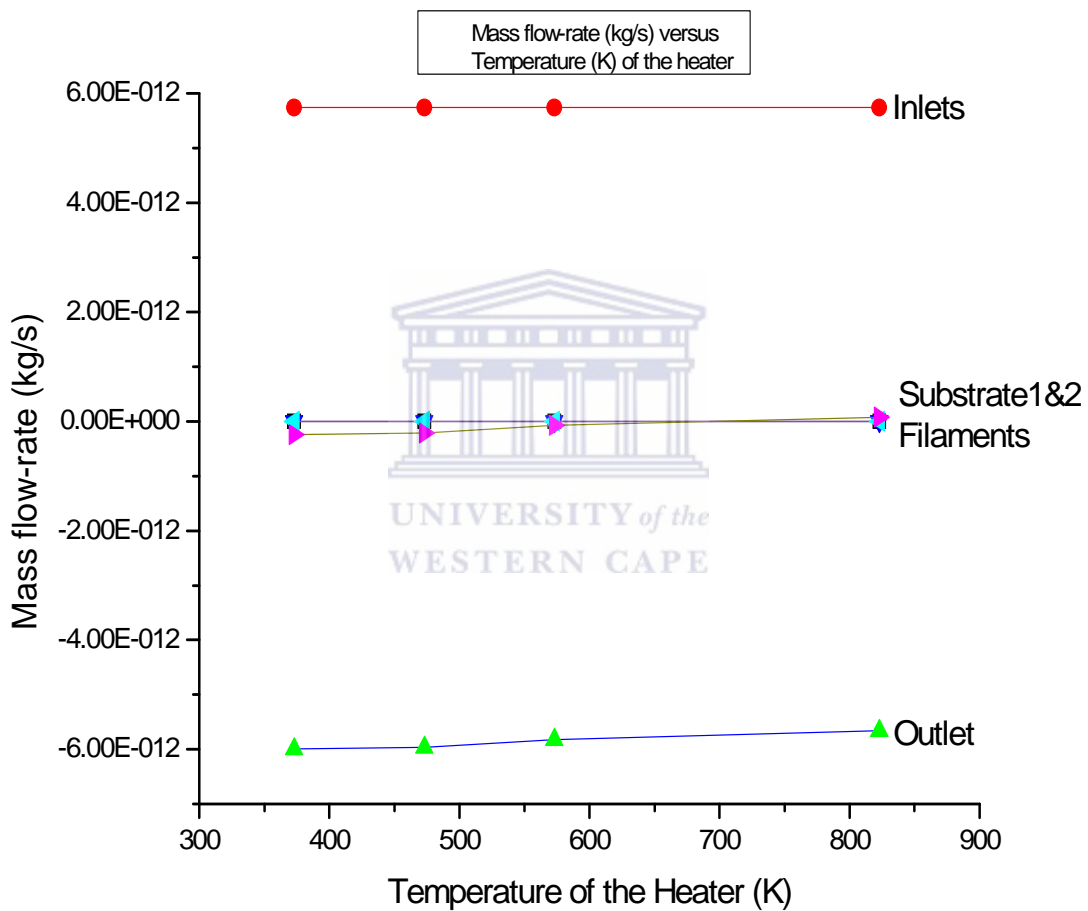
Name Of the Parts	Temperature of the Heater (°C)			
	100	200	300	550
<i>Filaments</i>	-2.12×10^{-17}	-4.17×10^{-17}	-8.61×10^{-17}	-6.32×10^{-16}
<i>Inlets</i>	5.74×10^{-12}	5.74×10^{-12}	5.74×10^{-12}	5.74×10^{-12}
<i>Outlet</i>	-5.99×10^{-12}	-5.96×10^{-12}	-5.82×10^{-12}	-5.66×10^{-12}
<i>Substrate1</i>	-9.35×10^{-20}	-2.15×10^{-19}	-4.81×10^{-19}	-5.01×10^{-18}
<i>Substrate2</i>	-2.52×10^{-19}	-4.51×10^{-19}	-8.32×10^{-19}	-6.49×10^{-18}
<i>Net Mass flow</i>	-2.45×10^{-13}	-2.17×10^{-13}	-7.57×10^{-14}	7.62×10^{-14}

From the Table 4.1, we can see from the four simulations that as the temperature of the heater are increased from 100 °C to 200 °C, 300 °C and 550 °C the mass flow rate flowing respectively around the filaments and the two substrates is decreasing. But the flow-rate of mass flowing out of the system through the outlet is increasing as the temperature of the heater is increased inside the chamber.

The temperature around the filaments of the HWCVD system at 1500 °C is slightly lower than the filament at 1600 °C. It is suggested that although chemical energy is released during the catalytic process, this is balanced by the removal of heat by the higher flow rate at the slightly lower temperature of the filament.

This is in agreement with practice where at higher flow rates and substrate temperatures the power to the filament had to be increased slightly to keep the

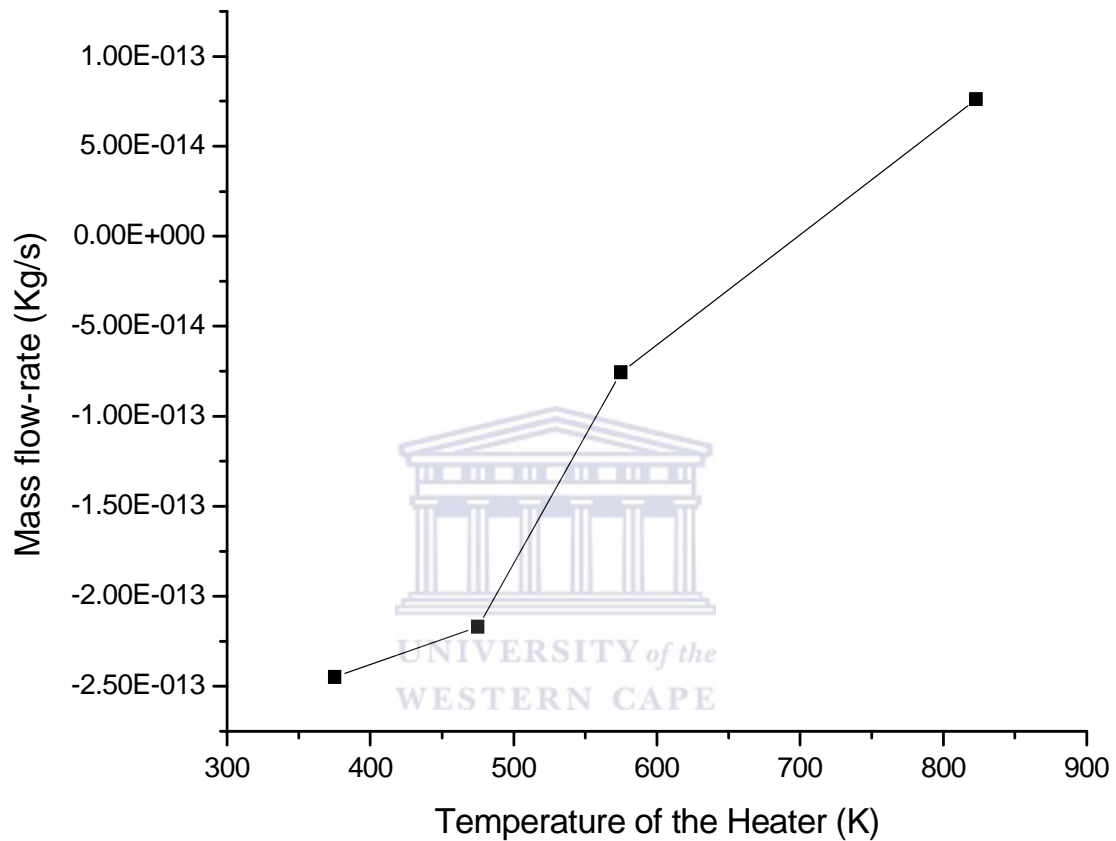
temperature at 1600 °C. The decreasing flow-rate at the outlet at increasing temperatures is suggested to be due to the faster removal rate of materials from the gas due to the higher deposition rate at the substrates. The results also show an increasing negative flow-rate at the filaments and substrate, this could be explained by the amount of material deposition on the filament and the substrates effective gas removal from the system.



Graph 4.1: A plot of the mass flow-rate on the filaments ,inlets, outlet and two substrates vs temperature of the heater for all four simulations.

The net flow-rate it is just the indication of the excess flow-rate flowing out of the system. This is only true at the lower temperatures at higher temperature it decreases

and at 550 °C it actually is less than coming in, meaning some of the gas remains behind. This would be due to the gas-atoms deposited at a high enough rates on the substrates to reduce the flow at the outlet.



Graph 4.2: A plot of the net mass flow-rate results around the filaments, inlet, outlet and the two substrates versus the temperature of the heater.

As we can see that the mass flow-rate flowing into the system for each simulation is about 5.74×10^{-12} kg/s and the one flowing out of the system for about three simulations, 100, 200 and 300 °C the outlet mass flow-rate is greater than the inlets flow rate. This is a small difference of about -2.46×10^{-13} which is about 4.3%. The plot in graph 4.1 shows the plot of the temperature of the heater all four simulations versus the mass flow-rate around the filaments, inlets and outlet. The net mass flow

rate results are also plotted in graph 4.2, this graph shows that the mass flow rate increases with the increasing temperature inside the HWCVD system. This is in agreement with the known results of the influence that the temperature inside the HWCVD system, as the temperature inside the system is increased the mass flow rate of the inside the deposition system also increases.

4.3 Surface Deposition-rate

The substrate heater temperature and the filament temperature inside the HWCVD system is very a very important process parameter affecting both the deposition rate and the properties of the deposited films.

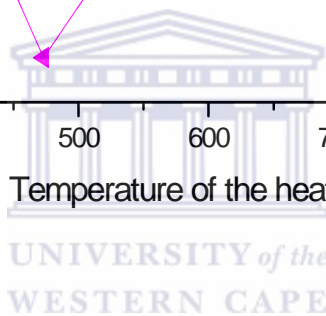
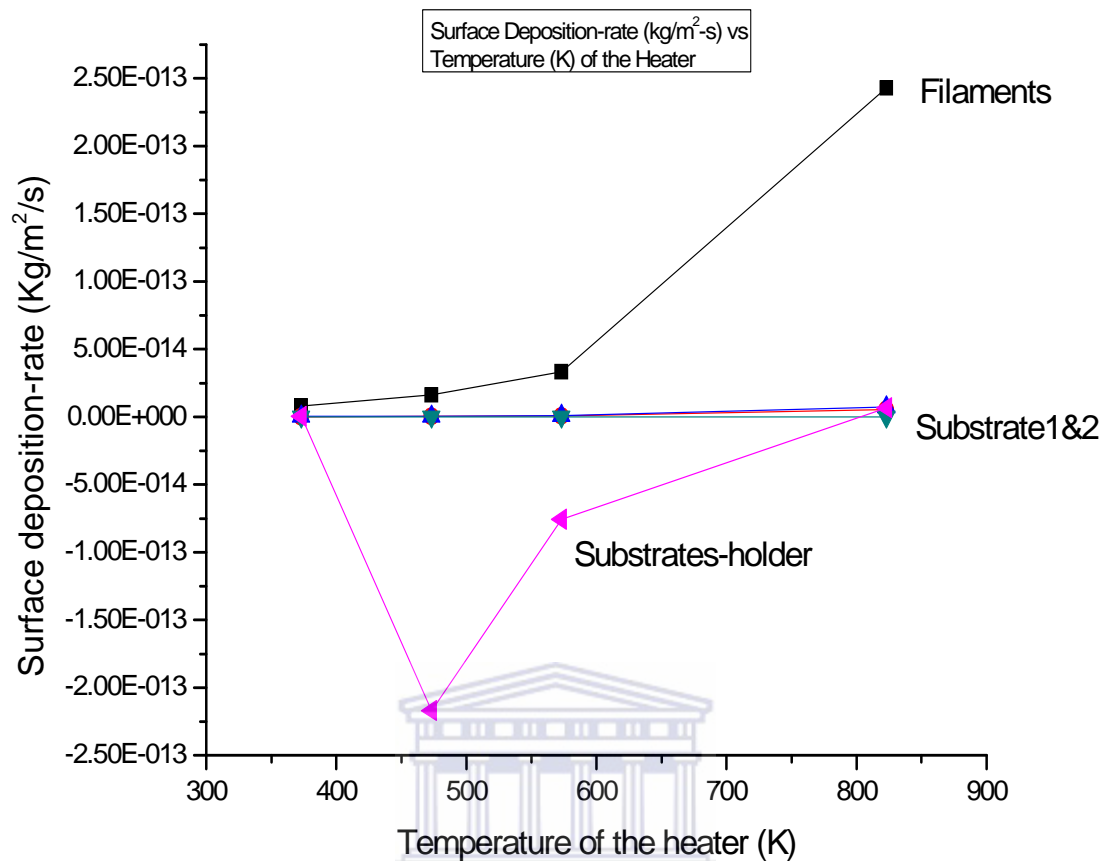
One way of increasing the deposition rate is to increase the breaking of the SiH_4 and H_2 molecules by increasing the temperature inside the HWCVD system. However, the use of higher temperatures in the HWCVD system increases the evaporation of tungsten from the filament, which, may lead to contamination of the growing film. The use of lower temperatures leads to the formation of tungsten silicate on the hot filament [38]. In section, the results of the surface deposition-rate are given.

Table 4.2: Surface deposition-rate results for all four simulations.

Name of the Parts	Temperatures of the heater			
	100 °C	200 °C	300 °C	550 °C
<i>Filaments</i>	8.16×10^{-15}	1.61×10^{-14}	3.32×10^{-14}	2.43×10^{-13}
<i>Substrate1</i>	1.04×10^{-16}	2.39×10^{-16}	5.34×10^{-16}	5.57×10^{-15}
<i>Substrate2</i>	2.81×10^{-16}	5.02×10^{-16}	9.24×10^{-16}	7.21×10^{-15}
<i>Sub-Holder</i>	2.75×10^{-18}	5.18×10^{-18}	9.97×10^{-18}	8.38×10^{-17}
<i>Net Deposition</i>	4.37×10^{-17}	8.61×10^{-17}	1.78×10^{-16}	1.31×10^{-15}

Table 4.2 above, shows the results for the surface deposition of the four simulations performed in this study. From the above results we can see that the surface deposition around the filaments, the two substrates and the substrates-holder increases with the increasing temperature of the heater for each simulation performed in this study. Thus this can be concluded that the deposition of the mixture of gases into the HWCVD system is influenced by the temperature around the system.

Below is the plot of the temperature of the heater for all four simulations versus the surface deposition-rate around the filaments, the two substrates and the substrates-holder.



Graph 4.3: A plot of the surface deposition-rate on the filaments, the two substrates and a substrates-holder vs temperatures of the heater.

The plot above shows the surface deposition-rate around the filaments, the two substrates and the substrates-holder for all four simulations by varying the temperature of the heater. From this plot, it can be seen that the surface deposition-rate increases with the increasing temperature of the heater in the HWCVD system.

This would mean that the deposition is influenced by the temperature of the system, with other parameters like the pressure inside the HWCVD system which is in agreement with known results [27].

4.4 Discussions

CFD is the analysis of a system involving fluid flow, heat transfer and associated phenomena such as chemical reactions by means of a computer-based simulation. In this study the mixture of the gas flow patterns inside the HWCVD system was modeled using CFD software package, FLUENT. The geometry of the HWCVD system was designed and meshed using the CAD design system called Gambit which is the first stage of the software package. In the second stage of the software (the Solver stage), most of the work was done by the computer itself; whereby using the discretizing scheme to express the governing equations in a discretized form for all mesh elements and discretizes the boundary equations appropriate at the boundary elements. In the solve stage the partial differential equations (Navier-Stokes equations) and the boundary conditions formulae are converted into a group of algebraic equation and the iteration procedure takes place. The simulations in this study converted after 6000-8000 iterations which took about 12 hours for the each simulation to converge and, this was due to the many parts that the HWCVD system contain and the finer mesh that was obtained.

The results given in 4.2 and 4.3 above are an indication of what influence or impact the mass flow-rate and the substrate flow-rate of the mixture of gases inside the HWCVD system. For one to come into a conclusion of having simulation results there are various procedure to be followed i.e. creating the geometry, changing the size of the mesh/grid of the geometry created, changing values for the parameters used in this study, setting-up boundary conditions, and re-running the simulation by performing the iteration. The results in table 4.2 shows that the parts which are closer to the heater and filaments have an increasing mass flow-rate as the temperature of the heater is increased and, this is in agreement with the known result [27, 38].

Chapter 5

SUMMARY AND CONCLUSION

A model based on computational fluid dynamics is, in principle, more precise and can include many features present in the fluid flow analysis; but requires much more computer time to run and needs a lot of information to model the boundary conditions. In performing a computational simulation using FLUENT, quality meshes should be generated to optimize the accuracy of the results calculated in the simulation. The mesh obtained in this study had Equisize skew (indication of the quality of the mesh) of 0.793051; which can be brought down to a smaller number leading to having very fine and much optimized mesh giving accurate results.

As outline under the table 4.2 and graph 4.2 in chapter 4, it can be concluded that the flow of the gas-flow patterns inside the hot-wire chemical vapor deposition system is influenced by the temperature, with other parameters like the pressure of the system and the rate in which the gas flows inside the system. In this study, we experienced a problem of having a simulation running for many hours due to the complex system we were modeling having parts with different shapes. It is again important to mention that in this study, there were no experimental results to compare the results obtained using the FLUENT software with. Most importantly, the simulations performed in this study gave an indication of how much the flow-rate and the deposition rate is affected by the temperature inside the HWCVD system.

In the appendix B there are plots of the path-lines obtained from the post-processor of FLUENT software, which shows how the gas flow patterns are distributed and flows throughout the system. These lines are an excellent tool in the FLUENT software to show how the mixture of the gas travels inside the HWCVD system. There are also contours of the temperature given in the appendix B, this is to show how the temperature of the heater which was varied in this study is distributed throughout the HWCVD system. From this tool it is shown how the parts which are closer to the heater and the filaments also had a higher temperature as compared to the parts which are far from the heated filament and heater.



REFERENCES

- [1] J.F. Douglas, J.M. Gasiorek, J.A. Swaffield, L.B. Jack, *Fluid mechanics, fifth edition*, (2005) 1-102.
- [2] H.K. Versteeg and W. Malalasekera, *An introduction to Computational Fluid Dynamics, The Finite Volume Methods*, (1995) 4-92.
- [3] C.J. Arendse, *Hydrogenated amorphous silicon; optical properties and hydrogen concentration*, MSc thesis, University of the Western Cape, (1998).
- [4] J. Lorenz, H.O. Kreiss, *Initial-Boundary value problems and the Navier-Stokes equations*, (1989) 1-18, 325-337.
- [5] B. Khanbabaie, A. Ghasemizad and H. Farajollahi, *CFD-calculation of Fluid Flow in VVER-1000 Reactor*, Journal of Applied Sciences 8 (5), (2008) 780-787.
- [6] K. Muralidah, T. Sundarajan, *Computational Fluid Flow and Heat Transfer, Kanpur Series of Advances Texts*, Narosa Publishing House, New Delhi, (1995).
- [7] H. Wiesmann, A.K. Gosh, T. McMahon, M. Strongin, J. Appl.Phys., **50** (5), (1979) 3752-3754.
- [8] A.H. Mahan, J. Carapella, B.P. Nelson, R.S. Crandall, I. Balberg, J. Appl.Phys., **69**, (1991) 6728.
- [9] Fluent Inc, *Fluent Version 6.3 Manual*, Centerra Resource Park, 10 Cavendish Court, Lebanon, New Hampshire, USA, (2006).
- [10] C. Hirsch, *Numerical Computation of Internal and External Flows*, Second Edition, (2007) 595-624.
- [11] R. Eymard, T. Gallovet, R. Habin, *Finite Volume Methods*, (2006) 4-93.

- [12] [WWW1] <http://www.grc.nasa.gov/WWW/k-12/airplane/nseqs.html>
[Accessed 12 April 2009].
- [13] A. Riddle, D. Carruthers, A. Sharpe, C. Mchugh, J. Stocker, *Comparison between FLUENT and ADMS for atmospheric dispersion modeling*, (2003).
- [14] Fluent Inc, *Gambit Version 2 Manuals*, Centerra Resource Park, 10 Cavendish Court, Lebanon, New Hampshire, USA, (2001).
- [15] S. Halindintwali, *A study of Hydrogenated nanocrystalline silicon thin films Deposited by hot-wire chemical vapour deposition (HWCVD)*, PhD thesis, University of the Western Cape, (2005).
- [16] S. Gu, C.N. Eastwick, K. Simmons, G. McCartney, *Computational Fluid Dynamics modeling of gas flow characteristics in a high-velocity oxy-fuel thermal spray system*, *Journal of thermal spray technology*, 10, (3), (2001) 461-469.
- [17] D.J. deKock, *Optimal Turnish Design Methodology in a Continuous Casting Process*, PhD thesis, University of Pretoria, (2005).
- [18] G.G Stokes, *On the Theories of Internal friction of fluid in Motion*, *Trans. Cambridge Phil.soc.*vol8, (1845) 287-305.
- [19] T. Frankiewicz, C.M. Lee, *Using CFD simulation to model fluid motion in Process vessels on fixed and floating platforms*, Natco Group, Houston, TX USA.
- [20] T.J. Jasinski, E.P. Childs, *Numerical Modeling Tools for chemical vapor deposition*, NASA Contractor Report 4480, Creare Inc. Hanover, New Hampshire, (1992) 39-67.

- [21] C.J. Brouckaert, T. Huang, C.A. Buckley, *Applications of Computational Fluid Dynamics Modeling in water treatment*, WRC Report No. 1075/1/05, (2005) 4-30.
- [22] C.J. Brouckaert, C.A. Buckley, *The application of Computational Fluid Dynamics to wastewater treatment plants*, WRC Report No. 648/1/02, (2005) 4-14.
- [23] G.F.J. Temple, *An Introduction to fluid dynamics*, Oxford at the Clarendon Press, (1958) 10-28.
- [24] G.H. Cottet, P.D. Koumoutsakos, *Vortex Methods, Theory and Practice*, (2000) 124-130.
- [25] G.L. Kaiser, T. Meersmann, J.W. Logan, A. Pines, *Visualization of gas flow and diffusion in porous media*, CA 94720, University of California, (2000).
- [26] K.K.S. Lau, H.G. Pryce Lewis, S.J. Limb, M.C. Kwan, K.K. Gleason, *Hot-wire chemical vapor deposition (HWCVD) of fluorocarbon and organo-silicon thin films*, Department of chemical engineering, Massachusetts Institute of Technology, Cambridge, MA, USA, volume 395, Issue 1-2, (2001) 288-291.
- [27] H.L. Duan, G.A. Zaharias, S.F. Bent, *MRS Symp. Proc.* **715**, (2002) A26.3.1.
- [28] S. Tange, K. Inouie, K. Konokura, M. Koski, *Thin Solid Films* **395**, (2001) 42.
- [29] H. Matsumura, *Japanese Journal of Applied Physics*, **25** (12), (1986) L949-L951.

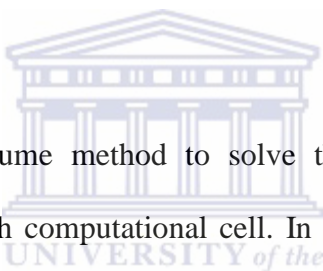
- [30] J. Doyle, R. Robertson, G.H. Lin, M.Z. He, A. Gallagher, *J. Appl. Phys.* **64** (6), (1988) 3215-3223.
- [31] J. Perrin, O. Leroy, M.C. Bordage, *Contrib. Plasma Phys.* **36**, (1996) 3.
- [32] J. Thangala, S. Vaddiraju, S. Malhota, V. Chakrapani, M.K. Sunkara, *A hot-wire chemical vapor deposition (HWCVD) method for metal oxide and their alloy nanowire arrays*, *Thin Solid Film* **517** (12), (2009) 3600-3605.
- [33] Q. Zhang, M. Zhu, L. Wang, F. Liu, *Influence of heated catalyzer on thermal distribution of substrate in HWCVD system*, *Thin Solid Film* **430**, (2003) 50-53.
- [34] C.J. Oliphant, C.J. Arendse, G.F. Malgas, D.E. Motaung, T.F.G. Muller, B.A. Julies, D. Knoesen, *Filament poisoning at typical carbon nanotube deposition condition by hot wire CVD*, *Journal of Material Science* **44** (10), 2610-2616.
- [35] T. Hadgu, S. W. Webb, M.T. Itamura, *Comparison of CFD Natural Convection and Conduction-only Models for Heat Transfer in the Yucca Mountain Project Drifts*, Albuquerque, New Mexico: Sandia National Laboratories (2004).
- [36] J. Tu, G.H. Yeon, C. Liu, *Computational Fluid dynamics: a practical approach*, First edition, (2008) 192-271.
- [37] J.H. Song, B.D. Ahn, S.D. Shin, N.M. Hwang, H.J. Kim, *Effect of wire temperature on the microstructural evolution of Si films in hot-wire chemical vapor deposition for digital display and photovoltaic devices*, *Solar energy Materials & Solar cells* **93**, (2009) 324-328.
- [38] B.P. Swain, R.O. Dusane, *Effect of filament temperature on HWCVD deposited a-SiC: H*, *Material Letters* **60**, (2006) 2915-2919.

APPENDICES

APPENDIX A

A.1 Introduction

The steady state segregated solver in FLUENT is used in this study. The segregated solver approach results in the governing equations being solved sequentially. An implicit linearization technique is applied in the segregated solution of the modeled equations previously described (in Chapter 2). Thus this results in a linear system of equations at each computational cell. The equations are coupled and non-linear; therefore, several iterations of the equation set are required to obtain a converged solution.



FLUENT uses a control-volume method to solve the governing equations. The equations are discrete for each computational cell. In applying this solution method the CFD simulation stores flow properties (e.g. dependent variables) at the cell centers. However, face values are required for the convection terms in the discretized equations. Face values are obtained by interpolation from the cell centers using a second-order upwind scheme for the momentum and energy equations and a first-order upwind scheme for the turbulence equations [35].

In this section a details CFD model (procedure followed in the FLUENT model at the solver stage) which was used in this study is given; and the calculation for the magnitude of the velocity of the gas flowing into the system, the heat flux of the filament and the species mass fraction which were used in the defining the boundary conditions in FLUENT.

Table A1: A detailed CFD model as used in this study.

Description	SETTING
Model	Pressure based, 3D steady state, laminar viscous model
Discretisation scheme	Second-order for pressure Second-order upwind for all other equations (momentum, energy etc.)
Glass properties: Specific Heat Density Thermal conductivity	700 J/kg/K 2579 kg/m ³ 1.05 W/m/K
Silicon properties: Specific Heat Density Thermal conductivity	700 J/kg/K 2329 kg/m ³ 130 W/m/K
Alumina properties: Specific Heat Density Thermal conductivity	800 J/kg/K 961 kg/m ³ 18 W/m/K
Tantalum properties: Specific Heat Density Thermal conductivity	140 J/kg/K 16690 kg/m ³ 57.5 W/m/K
Copper properties: Specific Heat Density Thermal conductivity	381 J/kg/K 8978 kg/m ³ 387.6 W/m/K
Inlet boundary condition: Velocity specification method Reference frame y-velocity inlet Inlet temperature	Components Absolute -0.18 300 K
Outlet boundary condition:	Zero gradient for all equations normal to boundary.
Filaments boundary conditions: Material name Thermal condition	Aluminum Heat flux
Heater boundary conditions: Material name	Steel
Wall boundary condition: Free stream temperature Other boundary walls	300 K Filaments-stand, Inlet pipe, Insulators, substrate 1, substrate 2 and substrate-holder.

A.2 Calculations of the magnitude of Inlet velocity

The total flow rate in the inlet is 60 sccm (this means that there will be a flow of 1 cm³ per second). The number of holes in the inlet-pipe is 7 (inlets).

- The radius of the inlets = 0.5 mm = 0.5 x 10⁻³ m per hole.
- The volume of the inlets is 1 cm³ = 1 x 10⁻⁶ m³, which then gives the flow-rate of the gases per second into the system to be: 1 x 10⁻⁶ m³/sec.

Therefore the velocity of the gas flowing into the HWCVD system is:

$$Velocity = \frac{flow - rate}{Area} = \frac{1 \times 10^{-6} m^3 / sec}{[\pi(0.5 \times 10^{-3} m)^2] \times 7} = 0.18 m / s$$

This velocity was used in setting the boundary conditions of the inlets in Fluent. This velocity of the inlet is on the negative y-direction (-y) in the geometry of the CVD system. Thus the boundary condition was set-up for the y-velocity to be -0.18 m/s.

A.3 Calculations for the heat flux of the filament

The total number of the filaments in the HWCVD system is seven (7) having the length of 11 mm and the radius of 0.05 mm. The temperature of the filaments of the HWCVD system is 1600°C. Having this information, the heat flux of the filaments was calculated as shown below and used in the simulation when setting the boundary conditions of the filaments in solver stage of fluent.

$$Area_{filaments} = 7 \times (2\pi rL) = 2.419 \times 10^{-3} m^2$$

The current flowing around the filament = 3.8 A \approx 4.0 A

The voltage applied over the filaments = 56 V \approx 60 V

Therefore the power flowing around the filaments is calculated as follows:-

$$Power = VI = 60V \times 4.0A = 240W$$

Then the Heat-flux of the filaments is given as:-

$$Heat - Flux = \frac{Power}{Area} = \frac{240W}{2.419 \times 10^{-3} m^2} = 99.21 \times 10^3 W / m^2$$

The calculations in (3.2.2) and (3.2.3) below were used in setting up the boundary conditions in FLUENT for the inlet magnitude velocity and the species mass fraction of the inlets.

A.4 Species Mass Fraction

The total flow-rate in the inlet of the HWCVD system used in this study is 60 *sccm*, in which is the total flow-rate of the two gases added together. As given in the nomenclature of this study, the *sccm* is the standard cubic centimeter which is the units for the flow rate of the gases inside the HWCVD system.

$$1\text{sccm} = 7.44 \times 10^{-7} \text{ mol / sec}$$

The flow-rate of *Hydrogen*(H_2) = 58.8sccm

Therefore the mass fraction for Hydrogen is:

$$\begin{aligned} H_2 &= 2 \text{ g / mol} \times 58.8\text{sccm} \times 7.44 \times 10^{-7} \text{ mol / sec} \\ &= \frac{8.75 \times 10^{-5} \text{ g / sec}}{1000\text{g}} \times 1\text{kg} = 8.75 \times 10^{-8} \text{ kg / sec} \end{aligned}$$

And the flow-rate for SiH_4 = 1.2sccm

Therefore, mass fraction of SiH_4 is calculated as follows:

$$\begin{aligned} SiH_4 &= \frac{1.2\text{sccm} \times [(28.09 \text{ g / mol}) + (4 \text{ g / mol})] \times 7.44 \times 10^{-7} \text{ mol / sec}}{1\text{sccm}} \\ &= \frac{2.86 \times 10^{-5} \text{ g / sec}}{1000\text{g}} \times 1\text{kg} = 2.86 \times 10^{-8} \text{ kg / sec} \end{aligned}$$

Then the percentage of the flow rate:

$$\text{Flow - Ratepercentage} = \frac{SiH_4}{H_2 + SiH_4} = \frac{2.86 \times 10^{-8} \text{ kg / sec}}{1.16 \times 10^{-7} \text{ kg / sec}} = 0.25$$

APPENDIX B

This appendix gives a detail flow results of the gas-flow patterns inside the HWCVD system. The appendix shows the temperature, velocity and the gas-flow distribution inside the system.

B.1 Contours and Path-lines

In figure B 1 and B2 shows the contour plots of the temperature around the walls of the deposition system. From the plots, it can be seen that the regions near to the filaments and the heater are hotter than the other parts. It can also be seen that above the heater and below the filaments stand are the cold dead zones of the deposition system from the plots.

In figure B3 and B4 is the pathlines colored by the temperature and the velocity respectively, giving a full overview of the flow of the gases inside the HWCVD system.

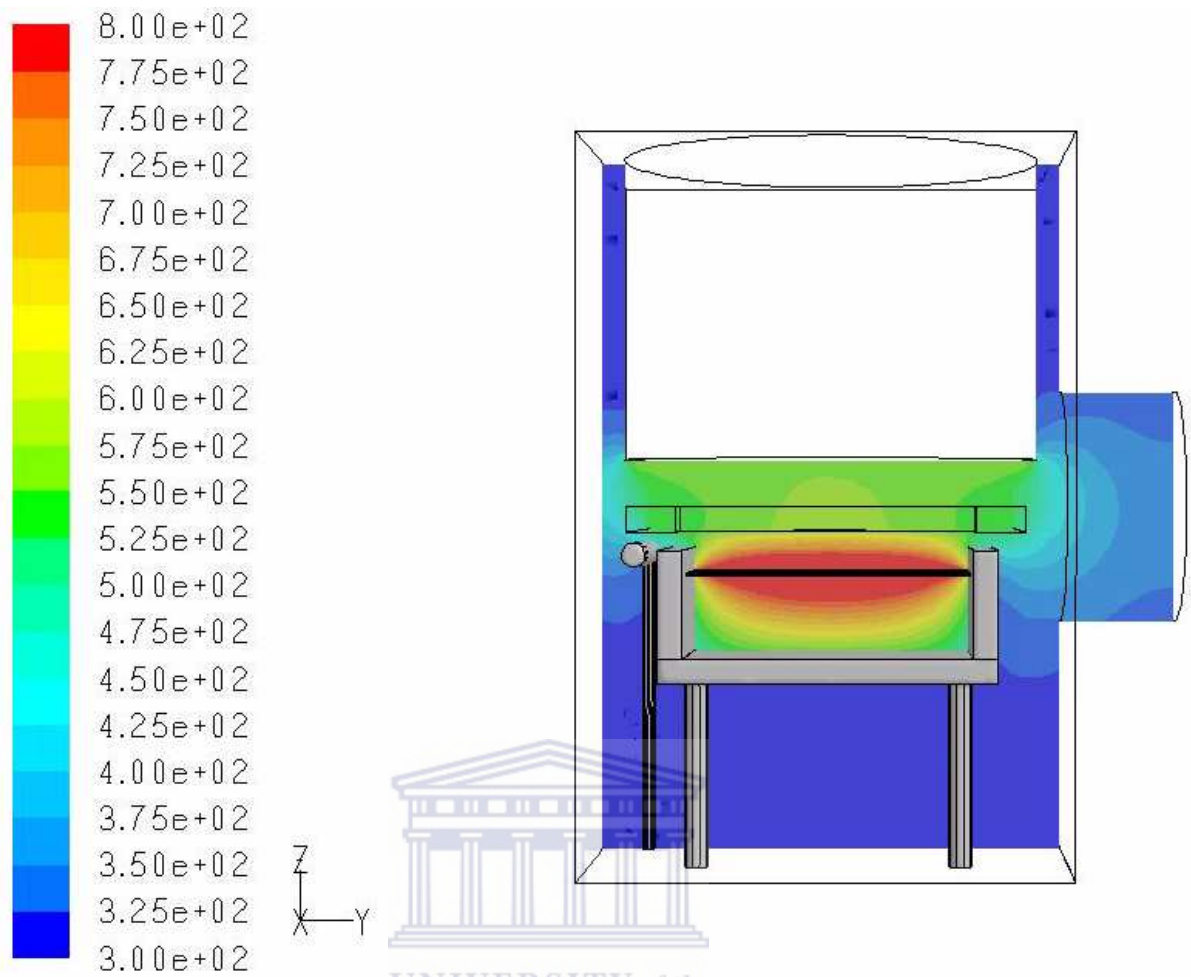


Figure B1: Temperature contours

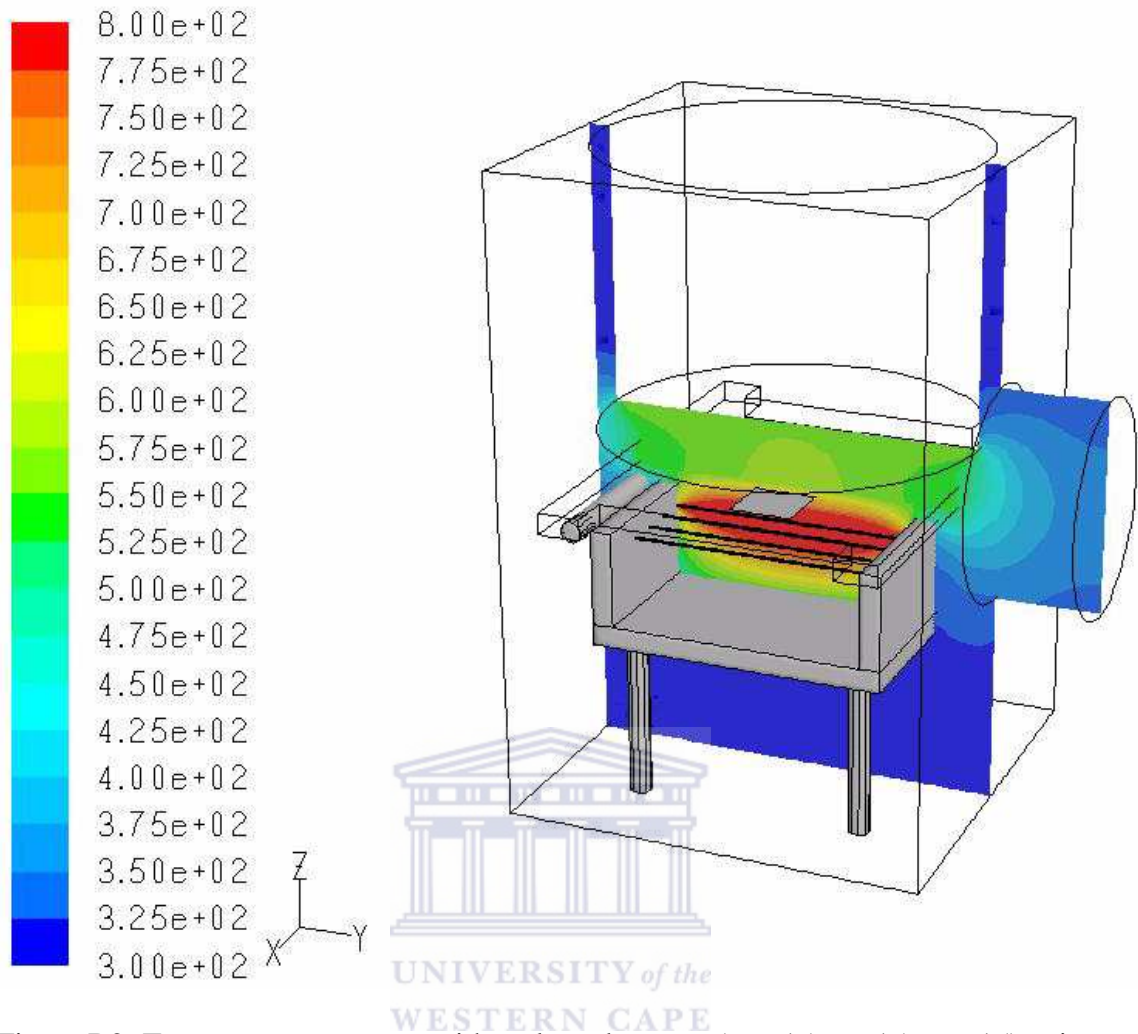


Figure B2: Temperature contours with a plane drawn at ($y_0=-15$, $y_1=15$, $y_2=-15$) axis.

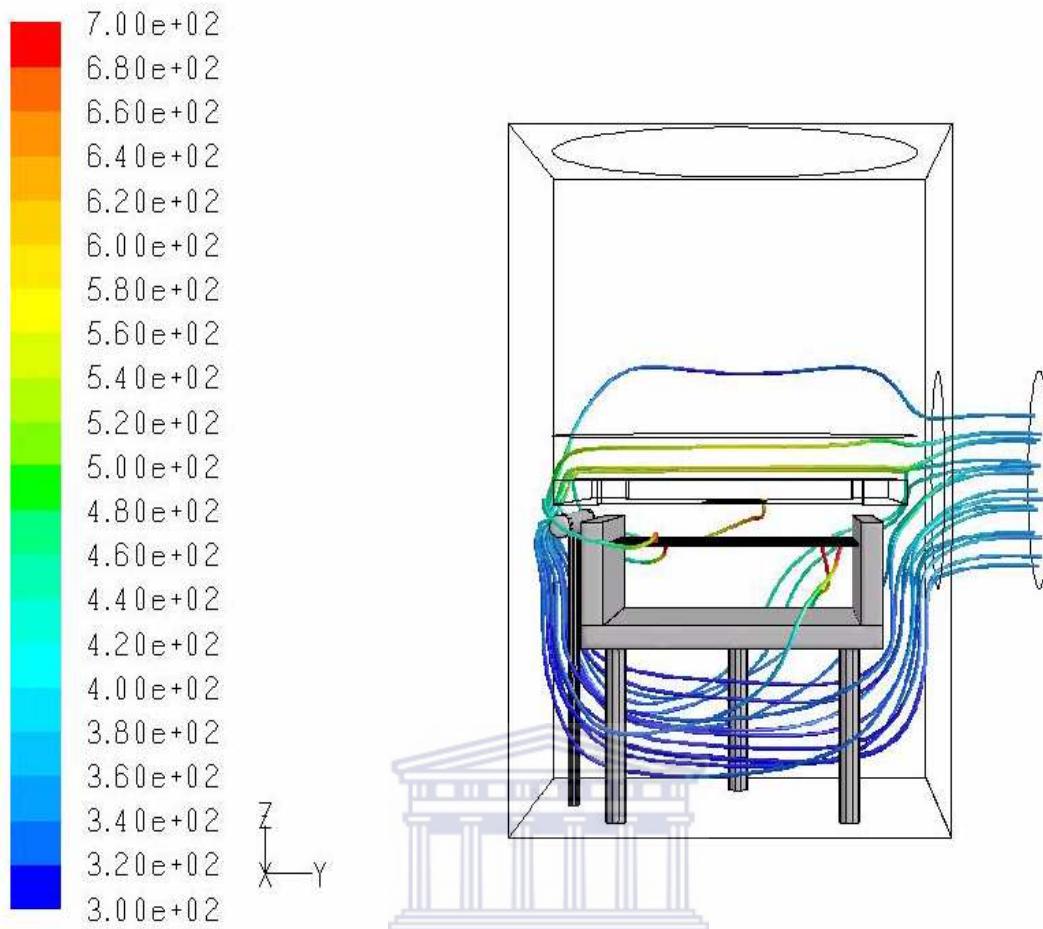


Figure B3: Path-lines colored by the Temperature.

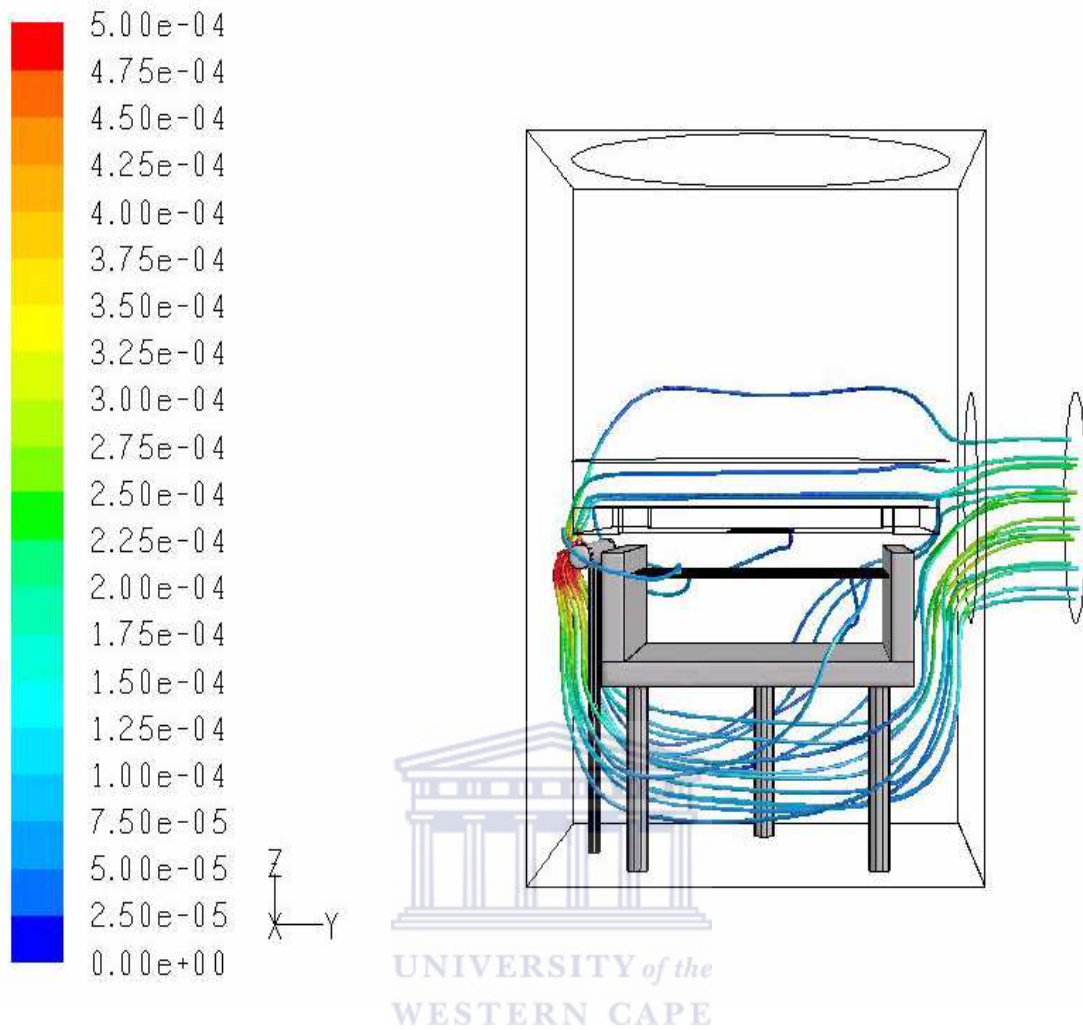


Figure B4: Path-lines colored by the velocity.