#### FINITE ELEMENT SIMULATIONS OF SHEAR AGGREGATION AS A MECHANISM

### TO FORM PLATINUM GROUP ELEMENTS (PGEs)

#### **IN DYKE-LIKE ORE BODIES**

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### ABSTRACT

This research describes a two-dimensional modelling effort of heat and mass transport in simplified intrusive models of sills and their feeder dykes. These simplified models resembled a complex intrusive system such as the Great Dyke of Zimbabwe. This study investigated the impact of variable geometry to transport processes in two ways. First the time evolution of heat and mass transport during cooling was investigated. Then emphasis was placed on the application of convective scavenging as a mechanism that leads to the formation of minerals of economic interest, in particular the Platinum Group Elements (PGEs). The Navier-Stokes equations employed generated regions of high shear within the magma where we expected enhanced collisions between the immiscible sulphide liquid particles and PGEs. These collisions scavenge PGEs from the primary melt, aggregate and concentrate it to form PGEs enrichment in zero shear zones. The PGEs scavenge; concentrate and 'glue' in zero shear zones in the early history of convection because of viscosity and dispersive pressure (Bagnold effect). The effect of increasing the geometry size enhances scavenging, creates bigger zero shear zones with dilute concentrate of PGEs but you get high shear near the roots of the dyke/sill where the concentration will not be dilute. The time evolution calculations show that increasing the size of the magma chamber results in stronger initial convection currents for large magma models than for small ones. However, convection takes, approximately the same time to cease for both models. The research concludes that the time evolution for convective heat transfer is dependent on the viscosity rather than on geometry size. However, conductive heat transfer to the e-folding temperature was almost six times as long for the large model (M4) than the small one (M2). Variable viscosity as a physical property was applied to models 2 and 4 only. Video

animations that simulate the cooling process for these models are enclosed in a CD at the back of this thesis. These simulations provide information with regard to the emplacement history and distribution of PGEs ore bodies. This will assist the reserve estimation and the location of economic minerals.

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## Symbols and Meanings

### Chapter 3

a <sub>1</sub> , a <sub>2</sub>	Viscosity coefficients (constants) for fitting equation (3.13)
	to data
$b_1, b_2$	Magma density coefficients (constants) for fitting equation (3.15)
	to data
A and B	Refers to constants for a particular solute (see equation 3.9)
C	Molar volume concentration of solid crystals in magma flow, see
	equation (3.8)
C <sub>0</sub>	Volume concentration of solid crystals at closest packing (~65%),
	see equation (3.8)
C <sub>p</sub>	The heat Capacity at constant pressure
d	Characteristic depth of fluid layer
$E_{\mu}$	The activation energy for viscous flow
g	The acceleration due to gravity
n	The parameter that measures the degree of non-Newtonian fluid
	behaviour, with $n \leq 1$
p	Pressure
r	Radius of spherical olivine crystal
Ra	Rayleigh number
Т	Temperature in degrees Kelvin
T <sub>0</sub>	Reference temperature (e.g., at which $\mu_{eff} = \mu_n$ )
$\overline{V}$	Magma velocity
β	Thermal expansion coefficients
Ŷ	A constant (= 1.50 for magma; = 1.35 for spheres of uniform size)
$\frac{d\overline{V}}{dy}$	Velocity gradient normal to the flow direction, see equation (3.5)

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	Chapter 4
το	The minimum stress (yield stress), see equation (3.5)
τ	Shear stress in the x-direction of the flow, see equation (3.5)
υ	Kinematic viscosity
	of=3.0
$\alpha_{v}$	The dimensionless coefficient for spherical solids of uniform size
θ	Temperature difference (e.g., T-T <sub>0</sub> )
	different molecular diffusivities, see equation (3.3)
Ks	Compositional diffusivity for a two- component system with
k	The thermal conductivity (assumed constant)
ĸŢ	Thermal diffusivity; = $\frac{k}{\rho C_p}$ , see equation (3.2)
Pcry	Density of the suspended solid crystals, equation (3.1)
	equation (3.1)
$\Delta \rho = \rho_{cry} - \rho_{liq}$	Density difference between the crystal and the liquid, see the
ρ <sub>n</sub>	Reference density ( $\rho_0$ ) in equation (3.15)
Pliq	Density of the magma
$\mu_n$	Nominal viscosity, see equation (3.13)
	C of suspended crystal load
$\mu_{eff}$	The effective viscosity of the magma containing a volume fraction
$\mu_0$	The viscosity of the magma without crystal content

E	The law of the wall constant in turbulence model, see equation
	(4.79)
Et	Total energy of the system, see equation (4.21)
$E_{\kappa}$	Turbulent kinetic energy (defined as ENKE in FLOTRAN), see
	equation (4.76)

.

E <sub>Kny</sub>	The near-wall turbulent kinetic energy, where nw is the near-wall
	node value, see equation (4.82)
е	Internal energy per unit mass
$ar{f}$	Force applied per unit volume on fluid particle, see equation (4.12)
G	The shear rate = $\frac{d\overline{V}}{dy}$ , see equation (4.89)
g	The vector acceleration due to gravity
Nu	The Nusselt number
$p_0$	Reference pressure, see equation (4.41)
<i>p</i> *	Hydrostatic pressure, see equation (4.41)
P <sub>v</sub>	The solid crystal dispersive pressure for viscous flow, see equation (4.86)
Q	The heat added to the system
$\overline{q}$	Heat flow per unit volume, see equation (4.25)
Gr	The Grashof number = $\frac{g\beta\theta d^3}{\upsilon}$ , see equation (4.58)
Pr	The Prandtl number = $\frac{v}{\kappa}$ , see equation (4.58)
r	The displacement of fluid element
u, v, w	The x, y, and z velocity components, respectively
$\overline{V_i^*V_j^*}$	Turbulent inertia tensor, see equation (4.68)
w	Work done on the fluid element, see equation (4.21)
V	Volume element
$\overline{V_0}$	Reference/initial velocity
$\overline{V}^*$	Velocity of the fluid during convective motions, equation (4.43)
$V_x^*$	The fluctuating component of velocity in the x-direction
$\langle V_x \rangle$	Mean component of velocity in the x- direction, equation (4.67)
$\overline{V}_{ ext{tan}}$ or $\overline{V}_{\delta}$	Velocity near -wall node parallel to the walls, see equation (4.80)

$\nabla$	Del operator for Cartesian coordinate system; = $\frac{\partial}{\partial x}\hat{i} + \frac{\partial}{\partial y}\hat{j} + \frac{\partial}{\partial z}\hat{k}$
Y <sup>+</sup>	Termed as YPLUS, is a non-dimensional distance from the wall,
	see equation (4.85)
$\frac{D}{Dt}$	The lagrangian operator, see equation (4.6)
$\delta_{ij}$	Kronecker delta function
τ <sub>y</sub>	Stress tensor, see equation (4.14)
€ <sub>ij</sub>	Strain rate of viscous deformation
δ	The boundary layer constant
$\mu_{l}$	Laminar viscosity, see equation (4.75)
$\mu_t$	Turbulent viscosity (eddy viscosity), see equation (4.75)
ρ*	Density measured relative to a static value, see equation (4.42)
$\Delta \rho = \rho - \rho_0$	The density difference relative to a static distribution
τ <sub>ij</sub>	Turbulent inertia terms;= $\mu \left( \frac{\partial V_i}{\partial x_j} + \frac{\partial V_j}{\partial x_i} \right) - \left( \frac{\rho V_i^* V_j^*}{Turbulent} \right)$ , equation
	(4.69)
K	The thermal diffusivity; $=\frac{k}{\rho C_p}$
3	Turbulent kinetic energy dissipation rate, see equation (4.77)
$\sigma_i$	Turbulence Prandtl number, it is a constant value assigned in
	FLOTRAN as default; $= 1.0$
٨	Linear concentration; = $\frac{1}{\left(\frac{C_0}{C}\right) - 1}$ ; the ratio of the solid diameter
	mean free distance between the solids, see equation (4.87)
T <sub>w</sub>	The wall shear stress, see equation (4.80)

 $\kappa_{w}$  The law of the wall dimensionless constant in turbulence models

Reynolds stress tensor, see equation (4.70)

### Chapter 5

$a_0, a_1$ and $a_2$	Undetermined coefficients, see equation (5.10)
D, B	Differential operators, see equations (5.1)
$C_{\phi}$	Transient and advection coefficient
dV	Volume element of the volume integral
$\{f\}$	Column matrix representing boundary conditions, equation (5.29)
$\left[G^{e} ight]$	The element conductance matrix, see equation (5.30)
[G]	The conductance matrix, see equation (5.29)
L	The subscript that denotes the nodal number $L = 1, 2, 3,, M$
М	Total number of nodes in problem domain $\Omega$
$n_x, n_y$	Components of the unit vector outwardly normal to $\Gamma$
$N_L(x,y)$	The basis function, see equation (5.3)
$R_{\Omega}$	The interior residual, see equation (5.2b)
$R_{\Gamma}$	Boundary residual, see equation (5.2b)
$S_{\phi}$	Source term.
$\overline{V}$	Velocity in components of x, y, z over the element $e$
$\overline{V}_s$	Fluid velocity tangential to the streamline, see equation (5.40)
W <sup>e</sup>	The weighting or shape function
$\frac{\partial^2 \phi_L}{\partial x^2} + \frac{\partial^2 \phi_L}{\partial y^2}$	The residual, see equation (5.7)
$\sum_{L}^{M} \left\{ \right\}$	The summation of terms from; $L = 1, 2, 3,, M$
Ω	The problem domain
Г	The Boundary of the problem domain ( $\Omega$ )
Γ	Diffusion coefficient

 $\sigma^{R}$ 

σ	Generalized variable representing a distance along the boundary in
	a counter-clockwise direction.
ø	The unknown nodal function defined within each element in terms
	of the basis function or interpolation over the problem domain
$\{\phi\}$	Column matrix for nodal functions
$\frac{\partial}{\partial t} \Big( \rho C_{\phi} \phi \Big)$	Transient term, see equation (5.32)
$\nabla \cdot \left( \rho C_{\phi} \phi \overline{V} \right)$	Advection/convection term, see equation (5.32)
$\nabla^2 (\Gamma_{\phi} \phi)$	Diffusion term, see equation (5.32)

#### **CHAPTER 1**

#### Introduction

#### 1.1 Thesis Description and Objectives

Wilson et al., (1989) provided geological evidence, which revealed the presence of two distinct, mineralized zones in the Great Dyke of Zimbabwe. One is the narrow and wellmineralized S1 zone. The second comprises the highly attenuated and sparsely mineralized zones S2 and S3. These pointed to two different controls on the same mechanism, which were not yet described for other layered intrusions. For example, Campbell et al. (1983) explained the Merensky and J-M Reefs to have been formed when one pulse of hot magma rose as a turbulent fountain into cooler resident magma. The latter has a density equivalent to or greater than the new primitive magma because of extensive crystallization of plagioclase (Wilson et al., 1989). These authors however, indicate this, the mechanism is not applicable to the Great Dyke, because at the level of the sulphide zones, plagioclase had not yet appeared on the liquidus and hence the residual liquid was less dense than the primitive magma. The above information indicates that there is at present no known knowledge to explain the processes involved in controlling the distribution and mineralization of PGE in the Great Dyke of Zimbabwe. Therefore, knowledge of associated magma transport and precipitation processes is desirable, since they may lead to more successful prediction of general distribution (Wilson et al., 1989). In spite of gravity studies done by Podmore and Wilson (1987) on the Great Dyke, much is still unknown about its actual shape. These are some of the reasons for this research effort. This study however should be viewed as a small component of a much larger project which aims at devising a computational model for the formation of ore deposits associated with igneous intrusions. The focus of this dissertation is to investigate the influence of variable geometry on convective scavenging (shear aggregation) and enrichment of Platinum Group Elements (PGEs) in the mineralized layers of the Great Dyke of Zimbabwe. This was accomplished by employing Computational Fluid Dynamics (CFD) with Finite Element Analysis (FEA) to examine the distribution of regions of high shear, and hence the location of economically

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interesting PGEs deposits. This should assist reserve estimation and location of mineral deposits.

#### 1.2 Methodology

The major hypothesis is this; the processes of interest are governed by the equations of fluid mechanics and other known physical laws. The laws are the continuity, Navier-Stokes and energy equations governing fluid flow and are described in chapter 4. These equations are solved with a robust finite element computer code, ANSYS 5.6. This code has been used to model the following geological transport processes:

- The convective temperature history of the magmatic fluid
- Mechanical models of magma chambers, which have provided insight regarding crystal settling, double diffusive convection and compositional convection.
- The cooling and solidification of magma chambers including the response of the surrounding country rock.

Currently, this study employs the code to model the following features.

- First, a simplified magma model of the Great Dyke of Zimbabwe was built and the geometry varied surrounded by a fixed country rock. This was done to examine the impact of geometry on the time evolution of both the convective and conductive heat and mass transport during cooling of the magma chamber.
- 2) Secondly, all the varied magma models geometries were used to examine the distribution of regions of high shear within the magma, and to identify the location of zones of zero shear, and hence the collection of PGEs. Computational turbulent analysis of this intrusive system was performed to generate regions of high shear. High shear results in enhanced collisions between the immiscible sulphide liquid particles and PGEs (Rice and von Gruenewaldt, 1994; 1995)
- 3) It is expected that these collisions scavenge PGEs from the primary melt, aggregate and concentrate and 'glues' them in place to form PGEs rich zones. The boundary layers are the most convenient regions to secure a high aggregation of PGEs (Rice and von Gruenewaldt, 1994; 1995). However, for dykes and sills the big phenocrysts concentrate and deposit at the center (Komar, 1972).

#### 1.3 PLATINUM GROUP ELEMENTS (PGEs) 1.3.1 Historical Preview:

The history of Platinum dates back to about 800 BC. The Egyptians used it, as evidenced by a casket, in the Louvre museum, bearing hieroglyphics made of an alloy containing several PGEs. There is also archeological evidence, which indicates that Indians of Ecuador and Colombians worked platinum many hundreds of years before the arrival of the Spanish explorers. The Spaniards discovered the source of platinum to be in the Chocco region of Colombia and the Incas recognized its rare quality because it never tarnished, thus making platinum a highly prized metal. They alloyed it with silver and gold. Platinum was intricately worked after the eighteen century, and then made into jewelry and other artful objects. This lead platinum to be greatly admired and used extensively by jewelers during the Art Deco movement in the 1920's and 1930's. It was during this era that Louis Cartier's first platinum watches were made. The scientific experimentation and investigation of the metal was first formally described in 1750 in a letter presented to the Royal Society, by Dr Williams Browningg in which he provided an account of the preliminary experiments carried out by himself and Charles Wood. However, it was not until 1804 that Williams Hyde Wollaston recognized that the native platinum did not just consist of one element, but also of palladium (Pd), rhodium (Rh), Iridium (Ir) and Osmium (Os). McDonald reviewed the most recent scientific history of platinum in 1982. Sir Humphry Davy in 1817 informed the Royal Society that platinum was a major catalyst, because it was able to promote a chemical reaction without itself undergoing any physical or chemical change. In 1830, Michael Faraday found that the metal was good for making glass since it did not contaminate the final product. George Matthey from 1825 to 1913, after working for 88 years on this was very instrumental in the refining and fabrication history of platinum from a laboratory scale operation into an important branch of industry.

#### 1.3.2 Chemistry of PGEs

The PGEs are divided into the light triad, which is: ruthenium (Ru), rhodium (Rh) and palladium (Pd) and the heavy triad: osmium (Os), iridium (Ir) and platinum (Pt). The light elements density is approximately half the density of the platinum triad. However, all six elements are generally unreactive. Strong alkaline oxidizing agents dissolve osmium but it is generally un-reactive in aqua regia (nitric/sulphuric acid mix), whereas both platinum and palladium dissolve in aqua regia. Platinum and palladium are soft and ductile which allows them to bend into different forms. Rhodium has excellent catalytic characteristics and when alloyed with platinum provides considerably superior properties at high temperatures. Ruthenium is hard and brittle and is difficult to work. Iridium retains its strength and corrosion resistance at very high temperatures and therefore makes very good crucibles. Osmium is of limited industrial use (Buchanan, 1988).

#### **1.3.3 PGEs Geology: Layered Intrusions**

A large magmatic body, which is emplaced into the earth's crust and cools slowly, is called a complex. During this slow cooling process the silicate, oxide and sulphide minerals crystallize and are thought to sink to the bottom of the magma chamber or form suspended loads with texturally distinctive layers. The removal of the more refractory minerals in this way depletes or enriches the residual melt. The magma changes composition continuously until solidification is complete. As a consequence, platinum group metals, nickel and copper, particularly when in the presence of a sulphide phase, can become sufficiently enriched to form layered mineralized horizons at predictable levels within the intrusion. Prime examples of such magmatic bodies are the Bushveld Complex, the Great Dyke of Zimbabwe, the Jimberlana Complex and the Stillwater Complex. This study concentrates on the formation of PGEs in the Great Dyke of Zimbabwe, which is the second largest PGE reserve.

#### 1.3.4 Technical and Industrial applications of PGE

#### 1.3. 4.1 Electronics

Before the emergence of solid-state devices, platinum-rhodium and palladium were widely used as an electro-mechanical switch for telephone exchanges in the telecommunication industry. Platinum, palladium and rhodium are also finding new uses in the electronic industry for thick-film integrated circuits printed onto ceramic substrates. These products are also used in the aviation industry where a high degree of reliability of materials is needed. Platinum group metal catalyst and current collectors are useful in fuel cells because of their high exchange current densities and their resistance to oxidation and dissolution under operating conditions (Buchanan, 1988).

#### 1.3.4.2 Vehicle Emission control (PGE) as a Catalyst

Carbon monoxide (CO), hydrocarbons (HC) and nitrogen oxide (NO<sub>x</sub>) are the principal polluting emissions from internal combustion engines. The effect of these pollutants can be reduced to a certain extent by the passing of hot gas through a catalytic converter, which consists of a porous honeycomb support coated with a thin layer of alloy of platinum, rhodium and palladium. The maximum performance of this catalyst is achieved by setting up a combination platinum-rhodium alloy with a ratio of 5:1. Such a three-way catalytic converter performs a dual function of reducing the nitrogen oxide (NOX) to nitrogen ( $N_2(gas)$ ) and oxygen ( $O_2(gas)$ ), while the hydrocarbons are oxidized to carbon dioxide and oxygen.

The removal of lead from petrol is an essential prerequisite because it reduces the hydrocarbons and nitrogen emission from exhaust fumes through the catalytic converters; For catalytic converters to operate at maximum efficiency lead free petrol is necessary (Buchanan, 1988).

#### 1.3.4.3 Jewelry and Dentistry

Platinum is used for jewelry for aesthetic reasons, as well for other qualities such as its potential to retain its lustre under extreme heat. When alloyed with iridium and ruthenium, it develops a high malleable strength, which allows the creation of the most desirable designs. The metal is ideal for the setting of precious stones because of its resistance to wear. In Japan two thirds of platinum goes into jewelry. However the demand for platinum in the west for jewelry has not been that satisfactory (Buchanan, 1988). In dentistry, platinum is replacing gold as a cheaper material for the fabrication of dental crowns and bridges. It is as inert as gold and mostly favoured by many state and private insurance schemes. Palladium is also replacing base metal for this purpose (Buchanan, 1988).

#### 1.3.4.4 The Chemical industry

The catalytic properties of PGEs have a particular application in the production of nitric acid. Nitric acid is one of the most important acids used in the production of nitrogen fertilizers and industrial explosives. Using the Ostwald process produces nitric acid; where ammonia is catalytically oxidized to nitrous oxide by finely woven platinum – rhodium alloy gauze.

#### 1.3.4.5 Glass Fibre production

Molten glass is drawn through platinum-rhodium alloy bushings which are uniquely able to maintain the fibre's size and shape under severe conditions.

#### 1.3.5 Marketing and Investment role

Most of South Africa's platinum and palladium is sold on contract at prices reflecting levels established on the free market, (see page 17, Buchanan, 1988; for tables). For The Rustenberg Platinum holdings (RPH) Johnson Matthey is the sole marketing agent for its products and Ayrton Metals Ltd acts as the selling agent for Impala's output of PGE. However, the Platinum ore reserves of the Great Dyke of Zimbabwe have not been fully exploited.

#### 1.4 Research Outline

This work calculates the transient and thermal behaviour of magmatic fluid under the constraint of variable magma geometry surrounded by a fixed solid (non-porous media) country rock geometry. It also calculates shear driven aggregation from calculated shear conditions within the magma chamber. By shear conditions is meant spatial variations in velocities, since high shear promotes aggregation, in that it enhances particle collision probability, which leads to greater particle collision rates (Rice and von Gruenewaldt, 1994,1995). This mechanism was applied in this research to model the collision between the immiscible sulphide liquid particles and PGEs in order to scavenge PGEs from the primary melt, to aggregate and concentrate them to form PGEs rich zones.

**Chapter 2:** This chapter provides a general description of the Great Dyke of Zimbabwe, its geology, layering, shape and cyclic units and sulphide mineralization and the distribution of the PGEs, particularly Platinum (Pt) and Palladium (Pd).

**Chapter 3:** A brief description is provided of the geological processes involved in modifying the composition of primary magmas and forming of igneous layering; namely, magmatic differentiation or fractional crystallization, gravitational settling, convection, double diffusive convection and igneous layering. This is followed by a brief outline of the physical properties of magmas.

Chapter 4: Provides a brief outline of the governing equations for Newtonian and incompressible fluid flow, buoyancy driven fluid flow, Boussinesq approximations, incompressible near- wall turbulence, shear driven aggregation, boundary layer theory, and thermal convection in magmas.

**Chapter 5:** Provides a basic introduction to the finite element techniques used by Ansys 5.6 to solve the Navier-Stokes equations. This section also discusses the theory solvers used for the transient incompressible flow.

**Chapter 6:** This section contains the physical properties used for modelling the magma chamber and solid country rock. This is followed by a list of boundary conditions and initial conditions of all the calculations done.

Chapter 7: All the simulation results are displayed in this section.

Chapter 8: Contains the discussions, conclusion and provides suggestions for future research.

#### CHAPTER 2 THE GREAT DYKE OF ZIMBABWE

#### 2.1 Introduction

Worst (1958,1960) presented the first comprehensive account of the Great Dyke and expanded on a mechanism for its emplacement, which was originally proposed by Hess (1950). Essentially magma was considered to have intruded through a primary fissure in each complex giving rise to successive horizontal layers. Worst (1958,1960) suggests that magmas ranged from mafic to ultramafic as the result of a primary differentiation process at depth and the sharp contacts between the layers were due to almost complete solidification of one pulse before the emplacement of the next surge of magma. A similar mechanism was suggested by Bichan (1969) and recognized that not all pulses crystallized completely before further injection of magma took place (Wilson, 1982). The major chromite and platinum-group element deposits of the Great Dyke evolve into large narrow elongate magma chambers, which are repeatedly replenished by these injections of primitive magma. The stratigraphic distribution and nature of these deposits have been attributed to variations in the replenishment process and to the fluid dynamic behaviour of the resident replenished magmas. However, the narrow width of the magma chamber led to a strong transverse heat gradient that imposed an additional constraint on crystallization (Prendergast and Wilson, 1989).

The Great Dyke of Zimbabwe is a major intrusion of mafic and ultramafic rocks and contains several economic minerals (Wilson and Tredoux, 1990). The Great Dyke lower ultramafic sequence is about 2000m thick and the overlaying center consist of remnants of gabbroic rocks from the mafic sequence with an approximate thickness of 1100m (Wilson *et al.*, 1989). It is the world's second largest reserve of Platinum-Group Elements (PGEs) after the Bushveld Complex (Naldrett and Wilson, 1990). The Chromite ore fields have been extensively mined for about 80 years, but the platinum-bearing horizons have not been fully exploited. The extent of the platinum-bearing zone of the Great Dyke and the revaluation of the precious metals market in recent years renewed interest in this deposit, and it is now recognized as a major PGE resource (Wilson and Tredoux, 1990).

The PGE enrichment has a close association with the sulphide mineralization. It is generally accepted that PGEs have a great sulphide affinity (Prendergast and Wilson, 1989; Wilson and Tredoux, 1990). All significant sulphide mineralization in the Great Dyke is hosted by the Pyroxenite No.1 (P1) layer at the top of the ultramafic sequence (Prendergast and Keays, 1989). The P1 section comprises one of the most complex packages of rock types in the Great Dyke and is also of major economic importance as it contains sulphide zones enriched in platinum (Prendergast and Wilson, 1989; Wilson and Tredoux, 1990). The sulphide-hosted PGE body requires:

(1) Enrichment of the PGE in the magma, which is most commonly, achieved by fractionation (Irvine et *al.*, 1983; Lee, 1989; Wilson and Tredoux, 1990).

(2) A mechanism for causing rapid crystallization of sulphide liquid together with efficient mixing of the segregated sulphide and the magma (Campbell and Barnes, 1984; Wilson and Tredoux, 1990)

The above information provides a good rationale to study the distribution of the sulphide - bearing layers, which will be discussed in later sections and in particular those zones which host the PGE.

#### 2.2 The Geology of the Great Dyke

The Great Dyke of Zimbabwe is 2575 Ma (Mukasa et al., 1998) old and 550 km in length cutting Archean granites and green stone belts of the Zimbabwe Craton. It is not a true Dyke in its present plane of erosion but a line of narrow layered mafic and ultramafic complexes (Prendergast, 1987). It is comprised of two major magma chambers (North and South chambers). The Mavuradona chamber, is is in the extreme north, see figure 2.1 (Prendergast, 1987; Wilson and Prendergast, 1989; Naldrett and Wilson, 1990). The width varies from 3 km to 11 km. The maximum thickness of the layered succession is 3.25 km (Wilson and Tredoux, 1990; Wilson and Chaumba, 1997). Stratigraphically the Great Dyke is divided into a lower Ultramafic sequence comprised of well developed cyclic units of Chromitite, Dunite, and Pyroxenite which is overlain by a succession of gabbroic rocks of the lower mafic succession (L M S). The LM S succession is the lowermost unit of the Mafic Sequence. Figure 2.2 shows the trumpet shaped transverse section of the Great Dyke, with the individual layers thinning

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**Figure 2.1:** The General locality map of the Great Dyke and a study area. The Great Dyke is located at (A) and (B), is the subdivision of the Great Dyke into chambers and a description of the Mafic and Ultramafic sequences. Location (C) which is the area outlined in map (B) is the part of the Darwendale sub chamber studied by the author. The picture is extracted from (Wilson, 1991)

away from the axis and eventually becoming incorporated into the layered Border Group which is parallel to the walls (Wilson and Prendergast, 1989; Wilson and Chaumba, 1997).



Figure 2.2: The transverse section of the Darwendale subchamber showing the synclinal shape of the layering (Wilson and Prendergast, 1989). This picture is extracted from (Naldrett and Wilson, 1990)

In the transverse section the layering in the Ultramafic Sequence is considered to be sigmoidal, resulting from the dip of the layering decreasing near the extreme margin and close to the axis (Wilson and Prendergast, 1989; Wilson, 1991).

This shape contrasts with the traditional vertical series of semi- circular cross- sections located at the axis and extending up to the margins of the border group (Worst, 1960; Wilson and Prendergast, 1989). It has important implications for the relative cooling history of the marginal and axial facies (Wilson, 1991). Worst (1960) considered the layering in its original form to have been subhorizontal with deformation occurring at high temperature both laterally and longitudinally in a graben structure which now defines the margins of the Great Dyke (Wilson, 1991).

Paleomagnetic studies on the Bushveld complex showed that rocks of the Main Zone were deformed by subsidence to their present position after magnetization. Similar studies on the Great Dyke indicated that no definite answer could be given as to whether magnetization preceded or followed the synclinal formation of the layering (Wilson, 1991). The mafic sequence and the upper layers of the ultramafic sequence probably extended upward beyond the present margins of the Dyke by several kilometers, but these lateral extensions are now entirely eroded along the length of the Great Dyke (Podmore and Wilson, 1987; Naldrett and Wilson, 1990). The mafic sequence, which has been preserved as remnants in the center of each sub chambers, is now extensively eroded. The elongate form provides a large surface area at the inclined wall/floor of the chamber. The attitude of the layering within the chamber is such that at higher levels the layers of rock overlap progressively onto the floor and wall of the chamber. Therefore a rock in the marginal environment is in close contact with the floor, whereas at the axis this same layer overlies a great thickness of ultramafic cumulates. These two environments within the P1 layer are referred to as the axial and marginal facies and there is a progressive gradation from one to the other. In the Darwendale Subchamber of the North Chamber, 2000m of the ultramafic Sequence are overlain by I120m of the Mafic Sequence (Wilson and Wilson, 1981; Naldrett and Wilson, 1990). The upper part of the Ultramafic Sequence is Websterite and this rock type is of importance because of its extensive development of Sulphide mineralization at its base (Wilson and Chaumba, 1997). The Sulphide mineralization is in some parts highly enriched in metals of the PEGs giving rise to economically viable ore bodies (Pendergast and Wilson, 1989; Prendergast and Keays, 1989; Wilson and Tredoux, 1990; Wilson and Chaumba, 1997).

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#### 2.3 Cyclic units

The cyclic units in the Great Dyke are thought by some authors to have been produced by the repeated injections of high magnesium (about 15% MgO) basaltic magma (Wilson, 1991), each of which underwent mixing with the resident magma and followed by fractionation and differentiation (Wilson and Tredoux, 1990). The nature of the cyclic units in the Bronzitite Succession differs between the two magma chambers. In the Darwendale subchamber cyclic layering is well developed in
the Ultramafic Sequence (Wilson, 1982, 1992) and 14 cyclic units are recognized (Naldrett and Wilson, 1990). Six major cyclic units in the North Chamber are recognized in the Bronzitite Succession of the Darwendale subcomplex, each is approximately 200m thick. In the South Chamber, there are 16 cyclic units, with each unit having a thickness of about 80m (Wilson, 1991). Figure (2.3A) indicates the division of the ultramafic sequence into a lower Dunite Succession and upper Bronzitite Succession with a well developed cyclic units 100 -200m thickness and the location of PGEs in the uppermost cyclic unit 1. The cyclic units in the dunite succession are defined by narrow chromitite layers, whereas those in the bronzitite succession show a complete progression from basal chromitite, through dunite, harzburgite and olivine bronzitite to a well developed bronzitite layer at the top, and as such represent an ideal unit of the Great Dyke (Wilson, 1982; Naldrett and Wilson, 1990; Wilson, 1991). The bronzitites are more resistant to weathering than the dunites (completely serpentized on surface) and they dominate the outcrop in many areas as a series of parallel ridges (Wilson, 1991). In the Darwendale and Sebakwe subchambers (fig 2.1), the layering plunges to the South and North respectively resulting in preservation of the remnant of the Mafic Sequence. Remnants of the Mafic Sequence are also preserved in the Musengezi, Selukwe and Wedza subchambers fig.2.3B (Wilson, 1991).

Cyclic unit1 is the topmost cyclic unit in figure (2.3A) and fig. (2.3B) is a larger view of cyclic unit 1 of the ultramafic sequence. Cyclic unit 1 marks the important transition from olivine and bronzite cumulates through websterites to gabbroic rocks of the mafic sequence (Wilson, 1991). This cyclic unit is also of major economic importance as it hosts both mineable chromitite layers and several zones of (PGE) mineralization (Prendergast, 1988; Prendergast and Wilson, 1989; Wilson, 1991). In the axis of the Darwendale Subchamber, Cyclic unit1 is 420m thick and is subdivided into six subunits on the basis of chromitite layers, chromite disseminations, and repeated lithologies (Prendergast and Wilson, 1989; Wilson and Prendergast, 1989; Wilson, 1991).

# 2.3.1 Cyclic unit 1: Stratigraphy and Lithologies

Six subunits are recognized in figure (2.3B), the four lower ones (1c-1f) are identified by basal concentrations of chromite and capped by granular harzburgite and olivine bronzitite. The poikilitic harzburgite is characterised by reaction and replacement of olivine and poikilitic enclosure by post



Figure 2.3: Stratigraphy of the Darwendale subchamber. Section. (A) Shows the major subdivisions and lithologies of the ultramafic sequence and (B) gives the detail of cyclic unit 1 in the axis of the subchamber showing subunit lithologies. Finally, section (C) shows details of cyclic unit1, near the west margin of the subchamber and a correlation with the axial section. This picture is extracted from (Wilson, 1982, 1991).

cumulus orthopyroxene. Granular harzburgite and olivine bronzitites [the distinction between these two rocks is the relative proportions of olivine and orthopyroxenes, see table1 in Wilson and Tredoux (1990)], which in turn overlie the poikilitic harzburgite, do not show olivine reaction (Wilson, and Tredoux, 1990). Chromitites in subunits 1c and 1d figure (2.3B) are of economic importance (Prendergast and Wilson, 1989) whereas those in the lower subunits are highly disseminated and generally less than a few centimeters in thickness (Wilson and Prendergast, 1987; Wilson and Tredoux, 1990). The sequence observed in each of the subunits is essentially similar to that of the major cyclic units in the ultramafic sequence, with olivine cumulates (mainly poikilitic harzburgite in cyclic unit 1) overlying the basal chromitite and the amount of orthopyroxene increasing upward (Wilson and Tredoux, 1990). Orthopyroxene becomes more abundant with increasing height and eventually attains cumulus status in the granular harzburgites and olivine bronzitites (Wilson and Tredoux, 1990).

The two top subunits (1a and 1b; in fig. 2.3B) are different from the lower ones in that pyroxene is the dominant mineral constituent and pyroxenites (bronzitite in subunit 1b and a 37 m thick websterite in subunit 1a) mark the top of the subunit (Wilson and Tredoux, 1990). This is successively overlain by a 3m thick olivine bronzitite, which marks the base of subunit 1a (Wilson, 1991). This olivine bronzitite at the base of subunit 1a dies out away from the axis of the Darwendale subchamber where it is replaced by a 30m thick bronzitite (Wilson, 1991), figure 2.3B, but the base of the subunit1 is still identified by a marked change in the grain size of the cumulus bronzite, and by the presence of small enclosed grains of chromite (Wilson and Tredoux, 1990). The main bronzitite layer of subunit 1b together with the olivine bronzitite, bronzitite, and websterite of subunit 1a are collectively referred to as the P1 pyroxenite layer figure 2.3C. In the P1 pyroxenite layer the bronzitite of subunit 1b once again overlies the olivine bronzitite and this is capped by websterite, which comprises cumulus augite and bronzite (Wilson and Tredoux, 1990).

Sulphide mineralization occurs through most of the upper half of the P1 pyroxenite succession in the Darwendale subchamber (Wilson and Tredoux, 1990). However, the narrow olivine bronzitite and olivine bearing bronzitite layers are included with the P1 bronzitite.

# 2.3.2 Sulphide mineralization and the distribution of Platinum (Pt) and Palladium (Pd)

Sulphides are present throughout the upper part of the subunits 1b and 1a of cyclic unit 1 and vary in modal abundance from the trace amounts (< 0.1 %) up to 8 percent (Wilson and Tredoux, 1990). The sulphide mineralization occurs as two zones within subunit 1a and one in subunit 1b in (fig.2.3B)



**Figure 2.4:** Diagrammatic representation of modeling results for progressive segregation of sulphide and Rayleigh fractionation of PGE's and Cu. A total of 0.012 % corresponds to a value between 3% and 10% pf amount of sulphide that can be dissolved in the Great Dyke-type at a level of cyclic unit 1. For comparison, see figures 3 and 4 in (Wilson *et al.*, 1989). The bases of sulphide zones have been modally gradational; with a 50% new magma which had been added to demonstrate replenishment of PGE's. This figure is an extraction from (Wilson *et al.*, 1989).

(Wilson and Tredoux, 1990). The Sulphide Zone 1, also called the Main Sulphide Zone (MSZ) (Bichan, 1969; Prendergast, 1988), is present in all subchambers at the same stratigraphic level (Prendergast and Wilson, 1989; Wilson *et al.*, 1989). The MSZ in the Darwendale consists of a 2-m thick interval with up to 10% disseminated sulphide and is located at, or just below, the bronzitite - websterite contact (Wilson *et al.*, 1989). The MSZ is further subdivided into a lower PGE subzone and an upper base metal sub zone. The disseminated sulphide zone in subunit 1b is referred to as the Lower Sulphide Zone (LSZ) (Wilson and Tredoux, 1990). Wilson *et al.*, (1989) introduced an informal terminology of S1, S2, etc., to allow flexibility on the nomenclature, and for sulphide zones of enhanced sulphide content, they used downward numbering in the sequence (Wilson and Tredoux, 1990). Zones with higher PGE contents related to these sulphide zones are identified by the informal terminology as M1 (i), M1 (ii), etc., (Wilson and Tredoux, 1990).

The Sulphide zone S1 is variable in thickness depending on the position in the subchamber relative to the geometric axis and extends from 1 to 5m below the websterite layer of subunit 1a. However, the pattern of distribution for sulphide is remarkably constant in all parts of the subchamber, although modal abundance is variable and also dependent on the position in the subchamber (Wilson and Tredoux, 1990). The general pattern of sulphide distribution in zone S1 is one of rapid development from initially very low levels (0.3 vol % to a maximum of up to 8vol %) over less than 2 m (Wilson and Tredoux, 1990). The modal abundance of sulphide then decreases upward in the succession through a series of diminishing peaks to less than 1 % over 2 to 5m, resulting in a vertical distribution which is overall highly asymmetric relative to the position of the maximum (Wilson and Tredoux, 1990).

The interval of maximum sulphide enrichment comprising the S1 zone is well defined over about 2m at the west margin of the Darwendale subchamber but becomes steadily wider toward the axis to a maximum of about 10m, where it is also much more disseminated, containing less than 3% sulphide (Wilson and Tredoux, 1990). The S2 zone in subunit 1a occurs between 5 and 15m below the base of S1. In the marginal facies the sulphide content does not exceed 1% and in the axis it is much lower that

0.3% (Wilson and Tredoux, 1990). The S3 zone is 15 to 20m wide and contains a maximum of about 1% sulphide. The lower sulphide zones of subunit 1b form a complex package of mineralized layers separated from the upper zones in subunit 1(a) by an interval containing very small amounts (< 0.1%) of sulphide.

There are a number of systematic variations in element concentrations and ratios that characterize each of the zones and subzones, which led them to conclude that each zone shares the same cyclicity (Naldrett, 1989). These aspects of the cyclicity are illustrated in figure 2.4. However, the model in figure 2.4 demonstrates the relative displacement of the peak values of Pt and Pd in the whole rock and the more rapid depletion of Pd in sulphide compared to Pt (Wilson *et al.*, 1989). The following observation was made.

(i) The concentrations of Pt and Pd increase with the amount of sulphide contained in the rocks.

(ii) The Pt and Pd content of the sulphides drops sharply as the percentage of the sulphide within the rock increases upward into each sulphide zone. The drop is distinctly sharper for Pd than Pt in the sulphide liquid (Naldrett, 1989). Because Pd is more rapidly depleted that Pt, suggests that Pd has the higher partition coefficient from the silicate melt into sulphide liquid (Wilson *et al.*, 1989).

(iii) Because of the more rapid drop of Pd than Pt, the Pd/(Pd +Pt) ratio also drops as the sulphide content increases at just above the base of a zone.

(iv) The Cu content of the sulphides (not shown in fig.2.4) remains constant and it shows no systematic trends; however, because of the drop in Pt the Cu/(Cu +1000 x Pt) ratio rises sharply to a value of 0.8 to 0.9 once the sulphide content of the rock increases at the base of a zone. See figure 2.4 in (Wilson *et al.*, 1989).

(v) The Pt and Pd contents of the sulphides remain low, once this drop has occurred within any given zone, but as the sulphide content of the rock decreases at the top of the zone, Pt and Pd in the sulphides starts increasing. As this occurs, the Pd/ (Pd + Pt) ratio raises rapidly to a value of about 0.6 and the Cu/(Cu+1,000 X Pt) ratio starts declining gently to a level out at a value between 0.2 and 0.4 (Naldrett, 1989). To produce the marked effect seen for Pt and Pd, the partition coefficients for these elements must be very high, about  $10^5$  (Wilson *et al.*, 1989). These conclusions were consistent with

the predictions of (Campbell *et al.*, 1983; Campbell and Barnes, 1984; Wilson *et al.*, 1989). To test for the fractionation model, the behaviour of Pt., Pd and Cu have been modeled for Rayleigh fractionation (Wilson *et al.*, 1989). There were no data available on the PGE content of the Great Dyke magma; so typical values for continental flood basalts of 10 ppb Pt and 5 ppb Pd were assumed for Pt (Barnes and Naldrett, 1985). These values were similar to those present at the early stages of the Bushveld and Stillwater complexes (Wilson *et al.*, 1989). Rajamani and Naldrett (1978) from the results of their experiments used the slope [i.e. D= (Weight percent of metal in sulphide liquid)/(Weight percent of metal in silicate liquid)], which is in any case, a form of the Nernst distribution law. They computed partition coefficients for Pt, Pd and Cu to be  $10^{4.5}$ ,  $10^5$  and 250, respectively. Trends for Pt and Pd distributions in the whole rock and the sulphides are reasonably matched between observations and the model in figure 4, with ratios Cu/(Cu+1000 x Pt) and Pd/(Pt + Pd) (Wilson *et al.*, 1989).

This last section has attempted to provide an understanding of the geochemistry of the Pt and Pd distribution and formation in the Great Dyke, necessary for future computational efforts.

### **CHAPTER 3**

### MAGMA PROCESSES AND THE PHYSICAL PROPERTIES

# **3.1 Introduction: Magma Processes**

Partial melting processes within the upper mantle generate the origin spectrum of primary basic and ultra basic magma. Once such magmas have segregated from their source region they undergo a variety of complex fractionation, mixing and contamination processes en route to the surface during transport and subsequent storage in high-level magma chambers (Freeman et al., 1986; Wilson, 1989). These processes are important in the production of diverse igneous rocks presently exposed to the earth surface. The upward progression of primary magmas starts from depths greater than 100km to less than 50km (Freeman et al., 1986; Wilson, 1989). The solidification of magma occurs over a temperature range; and the temperature during which crystallization starts occur is called the liquidus and that at which it completes crystallization solidus. The liquidus and the solidus are both pressure dependent and are sub parallel in the P-T space. Conveniently, figure 3.1 illustrates the solidification process in such magmas with assumed isobaric conditions to simplify calculations. When they enter the lower-density rocks, the rising basaltic magmas may reach a state of zero or negative buoyancy and pond, forming a magma chamber. The magma within the chamber cools by losing heat to the wall rocks (country rock) the temperature is then subsequently lowered to fall below the liquidus where crystallization begins. If the chamber is replenished by the injection of a new batch of primitive magma this may trigger an eruption of the porphyritic chamber magma (path A). Alternatively the magma batch may solidify completely with the crust, forming a plutonic or hypabyssal igneous rock (path B) (Wilson, 1989). Magma, which exists between its liquidus and solidus, is a mixture of crystal and liquid.



Figure 3.1: Schematic representation of the ascent path of basaltic magma to the surface in relation to its crystallization interval. This figure is extracted from (Freeman *et al.*, 1986; Wilson, 1989).

During cooling, one type of mineral crystallizes first and then upon further cooling it is joined by the crystallization of another type of mineral and so on. For basaltic systems the confining pressure exerts an important control on both the nature and the sequences of the minerals crystallizing (Wilson, 1989). Magma of basaltic composition will crystallize to form a basalt, dolerite, gabbro or eclogite depending upon the depth. However if a process operates within the magma body, which effectively separates the crystal and the liquid fractions and prevents equilibration then magmatic differentiation occurs within the chamber. This process is called *Fractional crystallization*.

### 3.1.1 Magma Differentiation/Fractional Crystallization

There is a general consensus amongst petrologists that the bulk of magmas are affected by crystal fractionation during their evolution (Huppert and Sparks, 1984). Fractional crystallization is a process whereby solid and liquid phases are separated. During this process different patterns of crystallization and melting produce different compositions from a uniform starting material. A number of authors believe the major mechanism involved is crystal settling. However, it is thought there is evidence that suggests that crystal settling is an inadequate explanation. Theoretical arguments by Bartlett (1969), Rice (1981) and Sparks et al. (1984) showed that settling is opposed by convection in large magma chambers and that the fluid motions can keep crystals in suspension. Rice (1981) and Sparks et al. (1984) suggested a process different from crystal settling to fractionate magmas. They drew upon the ability of double diffusive convection to segregate melt composition, calling this process "Convective Fractionation". Rice (1981) argued that convective fractionation is a process capable of generating highly differentiated liquids at the early stage of the evolution of the magma chamber. This process embraces a variety of convective phenomena caused by crystallization, which are described in laboratory experiments on aqueous solutions. Chen and Turner (1980) and McBirney (1980) noted that freezing at the walls left behind a fluid of different density, which could rise or sink through the magma. Chen called this "Compositional Convection".

A variety of mechanisms have been proposed to separate crystal and liquid fractions, this includes:

Crystal settling

Flow Separation

Filter pressing

• Incomplete reaction between crystals and the melt and the convective fraction to occur. This study will not discuss mechanisms such as flow separation, or filter pressing as the latter is beyond the scope of the present work. However, a brief discussion will be given about the other mechanisms. The successive fractional crystallization steps of the melt (i.e., crystallization) accounts for *Albite-rich plagioclase* as a final phase forming from the original *Anorthite-rich melt*. Plagioclase is a major mineral component of igneous rocks and its systematic change in composition is basic in classifying the range of intrusive from *granite to gabbro* and a range of extrusives from *rhyolite to basalts*. The plagioclase feldspars system ranges from Albite to Anorthite. Albite is a sodium aluminosilicate (NaAlSi<sub>3</sub>O<sub>8</sub>) and Anorthite is calcium Aluminosilicate (CaAl<sub>2</sub>Si<sub>2</sub>O<sub>8</sub>). The major difference between basalts and granites is as follows:

- Basalts are anorthite rich melts, whereas
- Granites are albite-rich plagioclase.

The magmatic differentiation process consists of the fractional crystallization, which moves the composition of the remaining melt to albite-rich plagioclase from anorthite- rich plagioclase. The basaltic magma is the starting material, which gradually differentiates to more silicic, melts by fractional crystallization (Freeman *et al.*, 1986; Wilson, 1989). To demonstrate this process Freeman *et al.* (1986) used plagioclase feldspars. The phase diagram in figure 3.2 gives a summary of many experimental results for the crystallizing of melts with composition corresponding to those of various members of the plagioclase series. The horizontal axis displays the chemical composition of the melt as the percentage of the two components, albite and anorthite and the crystallization temperatures are plotted on the vertical axis. The process starts with a melt of composition X (about 30% anorthite) heated to about  $1500^{\circ}$  C, and slowly allowed to cool.

# Steps of the crystallization process of plagioclase feldspar

• Initially, the melt of composition  $X_0$  (about 30 % anorthite) is at a temperature of about 1500°C and cools slowly to a temperature of about 1370°C to composition  $X_1$ , with no change in the liquid. At this point the first crystal composition  $C_1$  of plagioclase starts to form, consisting of about 70% of anorthite,

which is much higher than the original melt.

• As successive crystals are formed, the liquid becomes depleted in anorthite and then starts to move down the upper curve, to a composition at point  $X_2$ , which is less rich in anorthite. At this time the first crystals that were formed at  $C_1$ , become unstable with the liquid and then the composition moves down the lower curve to crystals of composition  $C_2$ .

• This process continues, the liquid now moves down the upper curve and the solid down the lower curve to a temperature of about  $1190^{\circ}$  C. The last drop of liquid (to about 5% anorthite) then forms crystals with the composition of the original melt X<sub>0</sub>. After that, the entire crystalline mass continues to cool without further change. Here the melt has crystallized into a plagioclase of the same original composition as the original melt. However,

• If crystals of composition  $C_2$  are withdrawn at this point before reacting, the liquid will change in composition to  $X_3$  and then the final crystal will be of composition  $C_3$ .

The reverse of this route occurs when a solid plagioclase is melted. The first liquid formed will be of the same composition as the last drop of liquid in the crystallization process. Magmas do not only crystallize to form plagioclase feldspars, they also produce mafic minerals such as, olivine, pyroxene, amphibole and biotite. During a slow cooling process all crystals react completely with the liquid. The olivine crystallizes first, the liquid then reaches a certain point where pyroxene starts to form and all olivine is then converted pyroxene. Melting and crystallization among these minerals is complex. Because they produce a discontinuous reaction series, these reactions occur between minerals of two definite compositions at a particular temperature rather than over a continuous range of compositions and temperatures, as compared with the plagioclase series. To demonstrate this process, the pseudoternary system of CaMgSi<sub>2</sub>O<sub>6</sub> (diopside)  $-Mg_2SiO_8$  (Forsterite)-CaAl<sub>2</sub>Si<sub>2</sub>O<sub>8</sub> (is provided in appendix A). During the process to differentiate magma, some portion of the crystals must be removed from the melt as they form; convective fractionation is one means (Rice, 1981). However, the mechanism, or gravitational settling is still under debate until such time as more experimental data is available to constrain this process.





### **3.1.2 Gravitational Settling**

In this process, crystals of greater densities than the liquid magma sink from the liquid as a result of gravity. However, if the density of the crystals is less than that of the liquid, the crystal float and the process is called *flotation*. *The* rates at which crystals settle depend on the following.

- Crystal size
- Viscosity of the liquid

• Density difference between liquid and the crystal for Newtonian fluids, the settling velocity  $\overline{V}$  for For Newtonian fluids, the settling velocity  $\overline{V}$  for small enough  $\overline{V}$  is governed by the Stokes law equation.

$$\overline{V} = \frac{2gr^2\Delta\rho}{9\mu} \qquad (3.1)$$

Wilson (1989) indicates that the time scales inferred from equation 3.1 are within the range of  $10^4 - 10^6$  years for large magmatic bodies. Equation (3.1) is only valid for Newtonian fluids and laminar flow and applicable to only basaltic magmas close to the liquidus. McBirney and Noyes (1979) found that partially crystallized basalts and those with Silicate (SiO<sub>2</sub>)-rich compositions inhibit crystal settling; therefore equation (3.1) is not valid. The theory of crystal settling in magmas is controversial. Some evidence cited in support of crystal settling theory is derived from field descriptions of high temperature mafic and ultramafic lava flows and thin sills, in which the denser olivine crystals are concentrated towards the base. For example, Wright (1971) supports this theory, with geochemical evidence; Wager and Brown (1967) took igneous layering as evidence of crystal settling.

However, Campbell (1977), Mc Birney and Noyes (1979), Irvine (1980a), Rice (1981), Sparks *et al.* (1984) and Turner and Campbell (1986) argue against the importance of crystal settling. The central theme of their argument is as follows.

There is a low probability of static conditions in magma chambers. This is because the convection will generally be turbulent which tends to hold crystals in suspension instead, of allowing them to settle.
Rice (1981) also argued that yield strength would greatly impede settling.

• Sparks *et al.* (1984) showed that, in general, the convective velocities are likely to be orders of magnitude greater than settling velocities.

# 3.1.3 Convection in magma chambers

# 3.1.3.1 Thermal Convection

Convection is a process that occurs when hot fluid is exposed to a colder environment or is heated from below. If heated from below, the fluid expands, becomes buoyant, rises to cool at the surface and then circulates back and down through the fluid. The pattern of circulation and heat transfer across the fluid can be predicted if the physical properties and applied temperature field are known. Convective motions in magmas can arise from compositional density differences as well (Shaw, 1965). The thermal aspects of convection are characterized by a dimension- less parameter known as the thermal Rayleigh number.

$$Ra_{T} = \frac{g\beta\,\theta d^{3}}{\kappa_{T}\upsilon} \tag{3.2}$$

Physically, the Rayleigh number for thermal convection in equation (3.2) is a function of the ratio of heat transferred by convection to that by conduction. The thermal convection for basaltic magma is highly turbulent in the early evolutionary stages for vertical dimensions greater than 1 km (i.e.  $Ra_T > 10^6$ ). Turbulence decreases as crystallization proceeds. This is due to an increase in viscosity with a decrease in temperature (Wilson, 1989). For large basaltic magmas thermal Rayleigh numbers range in excess of  $10^6$  up to  $10^{23}$  (Shaw, 1965; Bartlett, 1969;Rice, 1981). However, for 1km deep Rhyolitic, magmas a representative Rayleigh number may be as high as  $10^9$ . Such large values indicate that convection in magmas is vigorous and turbulent; Shaw (1965) indicated that prior to the 1970's all these applications concerning the convective theories of fluid processes for magma chambers were assumed as a one-component system. There is currently a flourishing research in this area.

# 3.1.3.2 Compositional Convection

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This type of convection occurs when there is a difference in density due to compositional change across a fluid layer of mean density  $\rho_0$  and thickness d. This density difference may be expressed as  $\rho_0\beta_s\Delta S$ , where  $\beta_s$  is the analogue of the coefficient of thermal expansion, but represents density change due to compositional change  $\Delta S$ . A dimension less parameter then expresses the convective motions in magmas arising because of compositional density difference. The compositional Rayleigh number,  $Ra_s$ .

$$Ra_s = \frac{g\beta_s \Delta Sd^3}{\kappa_s \upsilon}$$
(3.3)

Instead of using the compositional Rayleigh number, the ratio of the compositional to thermal Rayleigh number to yield the following relationship;

$$Q = \frac{\beta \Delta S}{\alpha \Delta \theta} \tag{3.4}$$

is used more frequently (Huppert and Sparks ,1984). The linear stability theory for convection applied to a single layer of fluid indicates that infinitesimal motions are initiated for Pr>>1 when Ra<sub>T</sub>-Ra<sub>S</sub> exceeds the critical value of order 10<sup>3</sup>. However, for a non- linear convection, the Rayleigh number difference Ra<sub>T</sub> - Ra<sub>S</sub> is much lower than the critical value and non-linear convection is also possible when there is a limit of very small diffusivity ratios  $\tau$ , and when the thermal Rayleigh number Ra<sub>T</sub> alone exceeds a critical value of 10<sup>3</sup>. However, the minimum Rayleigh number needed to maintain a series of layers still remains to be found but all laboratory experiments indicate that convecting layers easily form double-diffusive systems (Huppert and Sparks, 1984).

### 3.1.3.3 Double-Diffusive Convection

This is a property of multi-component fluids, whose individual components (including heat) have different diffusivities. This process occurs when the fluid becomes vertically stratified with respect to chemical composition and temperature. Sometimes there are opposing gradients of two components with different diffusivities. During this process, the system separates into a series of independent horizontal layers bounded by sharp diffusive interfaces, across which heat and chemical components are transported. Rice (1982) and Sparks et al. (1984) consider that this happens in silicate. The mechanism that controls this process is under debate. There are current theories that claim the settling of denser crystals is the mechanism responsible for separating the various components from the melt, which then may initiate double diffusive convection. However, laboratory experiments by Turner (1980) using crystallization from aqueous solutions to model the essential fluid dynamics process indicated another significant way by which chemical differentiation can be caused by relative motions between the crystal and the melt. This mechanism manifest that the growth of crystals of a denser component on a side wall boundary leaves behind the less dense, lighter fluid to rise to the top of the chamber in a boundary layer flow, which builds up a stable density gradient. The up flow in the boundary layer feeding up the lighter fluid to the top of the box results in the individual layers being pushed down with time. The crystals therefore do not remain in the same relation to the interfaces as they grow and any persistent layer structure, which is in the crystals, is then destroyed completely, but the interfaces remain the same. For cooling along the vertical wall, a number of experimental studies have shown that with crystallization along vertical walls, the heavier components are removed from the fluid, generating a boundary layer flow of depleted light solute (Turner and Gustafson, 1978; McBirney, 1980; Turner, 1980). A number of laboratory experiments have been set up to demonstrate double-diffusive convection, for which see (Huppert and Sparks, 1980a,b; Turner, 1980; Huppert and Turner, 1981a,b; Huppert and Sparks, 1984). Rice (1982) argued that many of these experiments lacked dynamic similitude. That is, they did not scale to magma chambers. Some of these experiments were performed in hopes of investigating the fluid dynamic aspects of open-system magma chambers for which there is an influx of primitive magma into a chamber containing more differentiated magma. These experiments attempted to illustrate an important principle relevant to some geological situations, specifically" A hot fluid can lie beneath a cold fluid if its composition is such that, it is denser" (Turner, 1980; Sparks *et al.*, 1980; Huppert and Sparks, 1980a,b; Huppert *et al.*, 1983; Huppert and Sparks, 1984). Such situations could occur in nature if primitive dense magma is emplaced into a chamber containing more differentiated melt. This would be similar to heavy hot brines or sulphide-bearing hydrothermal solutions discharged into the sea floor. In the case of magmas and brines, the cooling of such hot fluids leads to crystallization or precipitation, causing instabilities to develop which lead to the fluid layers mixing. With igneous processes, it is thought that the fluid layers of different compositions can coexist in the same chamber and evolve chemically as independent systems (Huppert *et al.*, 1982; Turner *et al.*, 1983). However, it is important to note that much of the double diffusive work that has been done was related to oceans and the quantitative and qualitative results obtained were for salty and fresh waters. "Therefore considerable caution is required when applying these results in a quantitatively way to geological systems" (Huppert *et al.*, 1983; Huppert and Sparks, 1984).

### 3.1.3.4 Convective Scavenging

Convective Scavenging (shear aggregation) is a process that causes particulate aggregation. This is brought about by creating shear conditions in fluids; that is, spatial variations in convective velocities in the flow in order to increase the frequency of particle collision amongst the particulate matter suspended therein. Shear aggregation is used as a common practice to concentrate and separate suspended particulate matter from fluids. The convective boundaries are of primary importance in securing such concentration, because the boundary layer is the region of greatest shear and where scavenging (of the most collision) takes place (Rice and von Gruenewaldt, 1994, 1995). In this study, the regions of high and zero shears are determined computationally. High shear regions lead to enhanced collisions between immiscible sulphide liquid particles and PGEs, and it is expected that these collision scavenge PGEs from the primary melt, aggregate, concentrate and 'locks' them place, to form PGEs enrichment in zero shear regions (Rice and von Gruenewaldt, 1994, 1995). Convective scavenging is applied to the igneous environment, because of the extremely high partitioning coefficient of PGEs into immiscible sulphide liquid.



**Figure 3.3** Demonstrates a double -diffusive convection process driven by shear aggregation. The shaded region in figure 3.3(a) indicates the boundary layers of double-diffusive convection with the arrows showing the flow directions. The vertical heat upflow warms up the bottom overlying layer causing localized upwellings in that layer. The bottom figure 3.3(b) shows details of the boundary layer. This picture is an extraction from Rice and vonGruenewaldt (1994,1995).

It is required that the R factor (Rfactor = mass silicate magma/mass sulphide liquid) be very large. The inability of pure diffusional transport of PGEs to secure effective scavenging is an inefficient concentration mechanism because it isolates the sulphide from additional PGEs in the reservoir and exhausts the local platinum content of the melt but its importance cannot be underestimated (Rice and von Gruenewaldt, 1994, 1995). This led to suggestions that turbulent mixing is involved (Rice and von Gruenewaldt, 1994; 1995). Campbell et al., (1983) in their attempt to explain the reason for the high PGEs concentrations in the Bushveld sulphides, suggested that because of the residence of the primary PGEs in a highly concentrated silicate melt, the concentration of the silicate melt was far more excessive than that of the sulphides which eventually hosted the PGEs; this means that the R factor must have been very large. They proposed a magma replenishment process whereby pulses of magma entering the magma chamber mixed turbulently with the host magma. The turbulence assured that sulphides were sufficiently exposed to the PGEs, in order to secure an effective high R factor. They also attributed the layering of the cyclic units to the arrival of new magma pulses in the chamber and early settling of the PGEs-rich suphides linking the PGEs -enriched layers with the base of the cyclic units. Another approach, by Rice and von Gruenewaldt (1995), showed that convective scavenging could form a 1m thick exploitable PGEs reef and /or chromitite layer from a column on the order of 300m thickness. When applying this concept to the Bushveld complex, Rice and von Gruenewaldt (1994) argued that it was more likely that the magma ponds rather than mixes. It is therefore more attractive to treat the magma chamber as a multi-layered double-diffusive convecting system as shown in fig.3.3 (a). This approach allowed drawing upon well-known processes in which disseminated material in a flow is scavenged and to which convection is fundamental. Furthermore, the division of each cyclic unit into layers of double-diffusive convection opens the possibility of placing chromitite layers in positions other than at the base of a cycle, as with the UG-2 chromitite and the UG-2 cycle (Rice and von Gruenewaldt, 1994). In this case, the boundary layer (separating layers of convection) would be the region where most of the PGEs partitions into sulphide liquid droplets (Rice and von Gruenewaldt, 1995). Viscosity of magmas is an important physical property that depends, amongst other things on strain rate, crystal content, volatile content and temperature. In figure 3.3(a) heat is transported upward through the fluid. As the fluid cools, its most refractory phases will crystallize out first and because of dispersive pressure, or the Bagnold effect, it will migrate into the boundary layer to

form two maxima in crystal content just inside the top and bottom of the boundary layer as shown in fig3.3 (b). Figure 3.3(b) shows, that the convective velocities are greatest on either side of the stagnation line (line of zero velocity) within the boundary layer that separates two layers of convection. When the boundary layer reaches approximately 65% crystal content, the flow experiences cohesive freezing, capturing into place the concentration profile of the more refractory components as shown in the upper left hand side of figure 3.3 (b) (Rice and von Gruenewaldt, 1994, 1995).

Rice and von Gruenewaldt (1995) conclude by emphasizing that shear aggregation is very efficient method to remove and concentrate compounds of interest from a melt. They calculated the time required to concentrate to ore-grade (e.g.; 6000-ppb of PGEs) within boundary layer approximately 1m thick from a body of magma 500m deep with PGEs content of 20ppb: an order of 100000 years. They further argue that, since convection is most vigorous when magma is warmest, half of this concentration would take place in the first 10000 years. This study seeks those regions of high shear in which convective scavenging would be most efficient for magma chamber of form similar to the Great Dyke of Zimbabwe and uses convective scavenging to model the PGE in the great Dyke of Zimbabwe.

## 3.1.4 Layered Igneous Rocks

Studies of layered igneous intrusions provide important constraints on the crystallization and chemical evolution of crustal magma chambers. These cumulate rocks preserve a continuous record of differentiation of the chamber magma. They may give fluxes of new batches of primitive magma mixing processes and wall rock (country rock) contamination effects. Some of these layered intrusions are immense. For example, the Precambrian Bushveld Intrusion in South Africa is exposed to over to an area of 65000 km<sup>2</sup> and has thickness of 7 km. The Tertiary Scorecard Intrusion in Greenland is relatively small, with an exposed area of 170km<sup>2</sup> and an estimated volume of 500km<sup>3</sup>. Table 3.1, shows some of the layered complexes that are of interest to this work (Campbell, 1977; Keays and Campbell, 1981, Maaløe, 1985).

# Table 3.1

Geology Complex	Area (km <sup>2</sup> )
Great Dyke Of Zimbabwe	300
Jimberlana Complex	unclear
Stillwater, United States	4400
Duluth, United States	4700
Dufek, Antarctica	unclear
Muskox, Canada	3500
Sudbury, Canada	1300

Most of these intrusions appear to be funnel shaped, although the diameter of the funnel relative to its height varies greatly and the layering is in general not parallel with the walls of the funnel (Wilson, 1989). Layering is usually defined by the variations in relative proportions of the constituent minerals. There may be gradational variations within a single layer, analogous to grading in sedimentary rocks. Tabular crystals such a plagioclase feldspar show marked preferred orientation within a layer, which has been considered suggestive of crystal settling. Naldrett *et al.*, (1987) postulated evolution of crystal-free liquid residua during the successive crystallization of olivine, orthopyroxene, plagioclase and clinopyroxene as cooling proceeds. However, in contrast to the crystal-free liquid model, Rice and

Eales (1995) calculated that the effect of suspended crystal load has considerable impact on magma density differences. This, has implications for the double-diffusive model of Irvine *et al.* (1983) in which the stratification of liquids within a magma chamber and the subsequent mixing of liquids rests critically upon small density differences between the crystal free A-type liquid density (2.592 g/cm<sup>3</sup>) and the crystal free U-type liquid density (2.577g/cm<sup>3</sup>). The mode of intrusion of fresh batches of magma therefore depends on the assumed densities of U-type and A-type liquids. The A- magma may be lighter or denser than the U-magma depending on its composition. Detailed studies of these cyclic layers has suggested to a number of workers that each unit cycle records the influx of new magma pulse and its subsequent mixing with the more differentiated chamber magma. During replenishment, hotter, denser, more primitive magma forms a layer at the base of the chamber, where it cools and crystallizes by exchanging heat across a double -diffusive interface with the more fractionated residual chamber magma (Campbell 1977, Irvine1980a). There is a considerable debate as to whether the accumulation of crystals at the bottom of layered intrusions is due to crystal settling or *in-situ* growth.

For the Skaergaard intrusion, Wager and Brown (1968), suppose that cyclic convection currents transported crystals growing near the roof zone down the walls and across the floor of the intrusion and because of their greater density, they settled out of the melt and are sorted hydraulically according to their size and density. Irvine (1980b) and McBirney and Noyes (1979) pointed out, there are significant deficiencies in these gravitational crystal-settling models and suggested that the settling of grains in magma may not be completely analogous process of clastic sedimentation. They, feel there is strong evidence favoring the *in situ* crystal growth.

• Carmichael *et al.* (1974) also suggested that the order of nucleation and growth of different minerals in basaltic magmas should be Fe-Ti oxides>olivine> clinopyroxene> plagioclase, thereby accounting for the sequence of minerals commonly occurring in micro- rhythmic stratiform intrusions. This would be the same sequence as that which would be produced by gravity sorting of equal- sized crystals. Hence during such *in situ* crystallization, the fluid in contact with the growing crystals convects away, followed by the development of compositional gradients in the magma chamber.

• Campbell (1977), McBirney and Noyes (1979), Irvine (1980a,b), Sparks et al., (1984), offered evidence that crystal settling is not a dominant process during crystallization in magma chambers

(Sparks *et al.*, 1984). Instead, crystals are thought to nucleate and grow *in situ* on the floor and the walls of the chamber (Turner and Campbell, 1986; Wilson, 1989). The above- mentioned argument, therefore, substantiates that fractional crystallization of the chamber is only possible if the depleted liquid is removed from contact with the growing crystals by a combination of diffusive and convective processes (Sparks *et al.*, 1984). Other authors emphasize, however, that such convection processes do not rule out the possibility of crystal settling in the evolution of basaltic magmas (Wilson, 1989).

#### 3.2 The Intrusion-Country Rock System

An intrusive -country rock system can be regarded as a chamber of molten magma which is injected in a single event over a very small time period into the earth's crust from the mantle, which upon slow cooling, solidifies into a crystalline or glassy igneous rock or a pluton. Heat from the cooling magma is then conducted into the country rock, which surrounds the chamber completely, thereby causing:

• Thermal convective transport of the groundwater contained within or

• Melting of the wall rock (country rock) due to heat of fusion released during the simultaneous crystallization of the magma itself (Wilson, 1989). This involves both mixing of the crustal and mantle partial melt and bulk assimilation. However, the bulk assimilation involves considerable input of heat, which must be supplied by the latent heat released during the simultaneous crystallization (Wilson, 1989). However, this study does not model either of the above, that is the groundwater or groundwater circulation and thermal fractures that result from the magmatic intrusions. The physical systems being modeled are:

1) The effect of changing the magma chamber shape on the time evolution of the convective transport of heat and mass during cooling of the magma and the heat conducted into the solid country rock, which completely surrounds the magma chamber.

2) The distributions of regions of high shear and shear aggregation within the magma should provide insight of the location of PGEs mineralization.

### **3.3 The Physical Properties of Magmas**

Most of the present information about the physical behavior of magmas is explained in terms of the properties of Silicon and Oxygen ions, which are the abundant components of igneous rocks. For details see Williams and Mc Birney (1979). Magma in its molten state is treated as fluid and certain physical properties of fluids are involved in any study of the fluid mechanics and the related process of momentum, mass and heat transfer in magma chambers. These properties include viscosity, density, thermal conductivity, heat capacity, diffusivity (Knudsen and Katz, 1958).

#### 3.3.1 Viscosity

Viscosity is an important factor governing both intrusive and extrusive processes. McBirney and Murase (1984) indicate that viscosity has an important influence on the mechanism of magmatic differentiation and crystal growth. Viscosity is defined as the ratio of shear stress to strain rate with the following mathematical formulation being:

$$\mu = \frac{\tau - \tau_0}{\left(\frac{du}{dy}\right)^n} \tag{3.5}$$

A more general definition of the viscosity  $\mu$  is  $\mu = \frac{d\tau}{d\gamma}$  where  $\gamma$  is the time rate of change of the shear stress. For simplicity, the definition in equation (3.5) will be used. The magma in its fluid state will be treated as a Newtonian fluid. Newtonian fluids have the following properties:

• They have no yield stress, i.e.  $(\tau_0 = 0)$ 

• Have a direct linear relationship between shear stress and strain rate, i.e. (n = 1), meaning that their shear stress tensor components are linear functions of the velocity gradient.

Thus equation (3.5) reduces to:

$$\tau = \mu \left( \frac{du}{dy} \right) \tag{3.6}$$

However, some non-Newtonian fluids but not all have the following properties: 1) A non-linear relationship between shear stress and strain rate, i.e.  $n \neq 1$ . 2) Minimum stress may be required initiate permanent deformation, i.e. the yield strength  $\tau_0 > 0$ . The shear stress tensor is a non-linear function of the velocity gradient

$$\tau = \mu \left( \frac{du}{dy} \right)^n + \tau_0 \,. \tag{3.7}$$

Murase and Mc Birney (1973) and McBirney and Murase (1984) point out that most magmas are nonnewtonian in their behaviour due to

1) The shear stress and strain rate that is not directly proportional, (n<1) below the liquidus, particularly when containing phenocrysts.

Below their liquidus, their shear stress and strain rate are not directly proportional, (n<1), particularly when they contain phenocrysts.

2) They are Bingham fluids or plastic fluids (i.e., they are silicate liquids with viscosities which have yield stresses and are time dependent). Bingham fluids have finite yield strength, such that below certain stresses the shear rate vanishes. This property was observed by, Shaw *et al.* (1968) in the basalts of the Hawaiian lava lake of Makaopuhi. Murase and McBirney (1973) also observed similar behaviour in Colombia River Basalts (CRB). These authors found that the stress required to produce a measurable shear increases with time, at a rate that increases as the temperature of the liquid falls below its liquidus. The change in viscosity with time is negligible above temperatures of 1245°C but increases tremendously at successive lower temperatures. The viscosities of magmatic fluids are also dependent on the following factors: crystal content; compositional dependence; temperature; pressure; water and time.

# 3.3.1.1 Crystal Content Dependence

Because most magmas in nature are at or below their liquidus they contain crystals in suspension, which affects viscosity as noted by McBirney and Murase (1984). Rice (1997a,b) points out that the effect of cohesive freezing (flow choking at about approximately 65% of the crystal content) will set the magma into place, preserving flow structure. For dilute crystal content, the Einstein viscosity law governs magmas.

$$\mu_{eff} = \mu_0 (1 - \gamma C)^{-2.5} \tag{3.8}$$

## 3.3.1.2 Compositional Dependence

The viscosity of silicic magma increases with increasing SiO<sub>2</sub> (silicate) content, because the silicate polymerizes the melt into long chains, which resist flow. For example, basalts with a silicate content of about 50% have a viscosity of about  $10^4$  Pas at a temperature of  $1000^{\circ}$ C and rhyolite with 72% silicate has a viscosity of  $10^{10}$  Pas at the same temperature, i.e.  $1000^{\circ}$ C (Williams and McBirney, 1979). For silicate melts, there is linear dependence on logarithmic viscosity composition. Jones and Doyle (1929) deduced a relationship for ionic solutions, expressed by.

$$\mu = \mu_0 \left( 1 + A\sqrt{C} + BC \right) \tag{3.9}$$

The  $A\sqrt{C}$  term accounts for increase in viscosity due to electrostatic attraction between oppositely charged nearest neighbour ions, always positive. The B coefficient is a characteristic for individual ions; it is either positive or negative. Bottinga and Weill (1972) modified equation (3.9) and proposed a model for compositional dependence of viscosity for silicate liquids, as follows:

$$\ln \mu = D_{SiO_2} + \sum_{j} \left( D_j - D_{SiO_2} \right) X_j$$
(3.10)

Where j indexes all the components other than  $SiO_2$  as the solvent of the silicate melt.

### 3.3.1.3 Temperature Dependence

Laboratory experimental results done on igneous rock by Williams and McBirney (1979) showed that the viscosity of magma drops with increase in temperature.

### Above the liquidus

The viscosity of most silicate melts above their liquidus has an inverse logarithmic variation with temperature according to the Arrhenius equation:

$$\mu = \mu_n e^B \tag{3.11}$$

Where  $B = E_{\mu}/RT$  is the exponential coefficient. Murase and McBirney (1973) explains that this activation energy is related to the proportion of bridging silicon and aluminium atoms, expressed by the ratio (Si+Al)/O for the melt.

### Below the liquidus

The viscosity of silicates below the liquidus increases more abruptly with a decrease in temperature than can be attributed to the Arrhenius equation (3.11). This viscosity increase with a drop in temperature is related to one of these two factors:

1) Increase in the strength of temporary fluctuating ionic bonds.

2) The crystallization of minerals, which is the more important factor.

For Colombia River Basalts (CRB), the crystallization temperatures begin around  $1275^{\circ}$ C and for Mount Hood Andesites (MHA) it is  $1240^{\circ}$ C. Different authors have different opinions regarding increasing viscosity with a drop in temperature. Shaw (1965) found that suspended crystal load to have a different effect from that predicted by equation (3.13). For T<T<sub>0</sub>, Adam and Gibbs (1965) modified

the Arrhenius equation to make it approximately equivalent to the Vogel- Tammann -Fulcher empirical equation of the form.

$$\mu = K \exp\left(\frac{E_{\mu}}{T - T_0}\right) \tag{3.12}$$

where K is the temperature dependent constant. This equation described successfully the temperature dependence of viscosity of many liquids. However, Bottinga and Weill (1972) found that neither of the above equations completely fitted measurements, possibly because their measurements were restricted to liquids. The Ansys FLOTRAN code can accomodate these viscosity formulations or can be employed to approximate the most accurate data available. FLOTRAN models the viscosity as a temperature dependent function as follows.

$$\mu = \mu_n \exp\left[a_1\left(\frac{1}{T} - \frac{1}{T_0}\right) + a_2\left(\frac{1}{T} - \frac{1}{T_0}\right)^2\right]$$
(3.13)

This relationship causes the viscosity to increase very rapidly as magma cools, hence replicating the solidification process, which occurs over a temperature range less than  $<<200^{\circ}$ C. The quadratic term allows equation (3.15) to take into account the crystal load during convection, and to approximate yield strength that is expected in the magma below the liquidus. The data was taken from experiments with magmas with different compositions, fitted to Equation (3.15) and were then plotted using Microsoft Excel (the 1997 version)- see figure 3.4.

### 3.3.1.4 Pressure Dependence

Little experimental work was done on pressure dependence until Waff (1975) theoretically predicted that the viscosities of Basaltic and Andesitic liquids decreased with increasing pressures at temperatures above the liquidus. However, recent findings show that with natural silicates the pressure load reduced

the viscosity of basaltic and andesitic melts at constant temperatures above the liquidus (Kushiro, 1980). The viscosity of basalts dropped from 17.0 Pas at atmospheric pressure to 4.0 Pas, 2.5 Pas, and 0.8 Pas at respective pressures of 15Kbar, 20Kbar and 30Kbar at respective depths of 45 km, 60km and 90 km (McBirney and Murase, 1984).

#### 3.3.1.5 Time Dependence

For temperatures below the initiation of crystallization, viscosity increases with time; if the magma is undisturbed, this continues for hours before reaching a steady value (Williams and McBirney, 1973). This increase of viscosity with time is thought to be due to the effect of an increase in population of suspended crystals.

# 3.3.1.6 Water Content Dependence

The effect of adding water to silica-rich composition decreases the viscosity of the magma. Water depolymerizes the silicate content by disrupting the Si-Al framework. The addition of water is, however, not pronounced for olivine and other silica -poor compositions (McBirney and Murase, 1979). The magmatic model used in this study is treated in the manner of unhydrous fluids; that is, not containing water.

### **3.3.2 Magma Densities**

Rice (1995) showed that a low crystal content, for example 1%, in a crystal would override the density changes solely because of thermal expansion or free melt evolution. Rice and Eales (1995) stressed that in other disciplines theoretical analyses of multiphase flows (for example, water and steam; air and sand; air and water or other particles; slurries; turbidity currents; sewage etc) treated the density of the total flow as dependent on the densities of both transporting fluid and its load. This practice of including the particulate load in determining the density of multiphase flow carries over into the physics of geological sedimentation. From practical engineering evidence Rice and Eales (1995) concluded that the

stratification of magmas within a chamber or at the level of neutral buoyancy to which plumes rise may be controlled by the relative crystal loads of resident newly injected magmas rather than by small density changes arising out of temperature difference or compositional changes accompanying fractionation. In summary, the density  $\rho$  of magmatic fluid varies mainly with temperature, chemical composition and crystal load content. All of which have temperature dependence density of magmatic flow. It can therefore simply be expressed as a function of temperature and pressure.

$$\rho = \rho(T, p) \tag{3.14}$$

For incompressible fluids, variations in pressure do not cause significant differences compared to the temperature variations. The general form of the temperature dependent density is of the second order; as used by Ansys, in the FLOTRAN code, it is expressed as:

$$\rho(T) = \rho_n + b_1 (T - T_0) + b_2 (T - T_0)^2 \qquad (3.15)$$

The second order term:  $b_2(T - T_0)^2$  can be made to account for the rapid increase in density with increased crystal load during cooling. The densities of most common igneous rocks for instance mafic basalts are 2800 kg/m<sup>3</sup> and for rhyolites 2200 kg/m<sup>3</sup>.

### 3.3.3 Magma Temperatures

McBirney and Murase (1979) indicate that the temperatures for most erupting magmas fall between the ranges 800°C -1200°C.

- Low temperature values are only observed between differentiated, carbonitive and felsic magmas.
- · High temperature eruptions are confined to basalts

The temperature range for a typical basalt, for example Colombia River Basalts (CRB) is between  $800^{\circ}$ C -  $1100^{\circ}$ C; temperatures above  $1200^{\circ}$ C are rarely observed. This thesis models the density data by using the curve- fit formula, equation (3.15).

# 3.3.4 Thermal Conductivity and Heat Capacity

In the present study the temperature ranges are modelled where the temperature dependence is small enough to treat the thermal conductivity as a constant:  $k = 2.0J.m^{-1}.s^{-1}.K^{-1}$ . Basaltic magma is the melt used in this study with upper temperature limit of  $1200^{\circ}$ C. For this work, C = 1200J. K<sup>-1</sup>.s<sup>-1</sup> is also treated as a constant. At this stage, single-phase fluid flows with no enthalpy changes are being modelled.



**Figure 3.4**: Log Viscosity in (Pas) versus Temperature in Kelvin (K) curve for Colombia River Basalts. The data was extracted from experiments performed by Bottinga and Weill (1972).



**Figure 3.5:** The Density  $(kg/m^3)$  versus Temperature in (K) curve for Colombia River Basalts (CRB). The data used was extracted from the experiments performed by Bottinga, Weill and Richett (1982).

# **CHAPTER 4**

# THE GOVERNING EQUATIONS FOR MAGMA AND SHEAR AGGREGATION

# 4.1 Introduction: The Governing Equations

This section provides some theoretical background on the conservation laws governing material transport. We apply these conservation laws to fluids in which case they are known as the Navier-Stokes equations (which includes heat transfer). The derivation of these equations may be found in (White, 1991). This study treats magma as a Newtonian fluid. These equations are:

•The Continuity equation: conservation of mass

• The Navier- Stokes equation: conservation of Momentum

•The Conservation of Energy equation: the first law of thermodynamics (White, 1991) The unknown variables that must be determined from these three basic equations are the velocity field  $\overline{V}$ , thermodynamic pressure (P) and the temperature (T). White (1991) regards the thermodynamic pressure (p) and temperature (T) as the two required independent thermodynamic variables. However, the final form of the conservation equations also contains four other dependent thermodynamic variables: the density ( $\rho$ ), enthalpy (h), or the internal energy (e) and the two-transport properties viscosity ( $\mu$ ) and thermal conductivity (k). The latter properties may be pressure (p) and temperature (T) dependent. Their variations with independent thermodynamic variables, pressure (p) and absolute temperature (T), are related by the following equations of state:

for density

$$\rho = \rho(p, T)$$

(4.1)

heat, or energy

$$\mathbf{e} = \mathbf{e} \left( \mathbf{p}, \mathbf{T} \right) \tag{4.2}$$

viscosity

$$\mu = \mu (\mathbf{p}, \mathbf{T}) \tag{4.3}$$

thermal conductivity

$$k = k (\mathbf{p}, \mathbf{T}) \tag{4.4}$$

However in this work the state equation (4.4) is treated as constant. The enthalpy (h) or intenal energy (e) is proportional to the temperature (T) by the following relationship (White, 1991; Currie, 1993).

$$e = C_p T \tag{4.5}$$

 $C_p$ , the specific heat, is assumed constant in the present FLOTRAN calculations of magmatic intrusions. The governing equations for fluid flow make possible the determination of the convective velocity field  $\overline{V}$ , the pressure P, and the temperature T at every point in the flow regime. These considerations are applied to a fluid that is assumed to be of uniform homogeneous composition. That is, no account is taken of multi-component reacting fluids such as:

Conservation of species

· Laws of chemical reactions

# **4.1.1 The Continuity Equation**

The mathematical equivalence of this statement of mass conservation is:

$$\frac{D}{Dt} \int_{V} \rho dV = 0 \tag{4.6}$$
The Reynolds transport theorem in tensor notation is expressed as (Currie, 1993).

$$\frac{D}{Dt}\int_{V}\alpha dV = \int_{V} \left[\frac{\partial\alpha}{\partial t} + \frac{\partial}{\partial x_{k}}(\alpha V_{k})\right] dV$$
(4.7)

Where  $\alpha$  is the fluid property, equation (4.7) transforms equation (4.6) which is a combination of the arbitrary control volume and the Lagragian into an equivalent expression involving integrals of Eularian derivatives, hence equation (4.6) now becomes.

$$\int \left[\frac{\partial \rho}{\partial t} + \frac{\partial}{\partial x_{*}}(\rho V_{*})\right] dV = 0$$
(4.8)

Where the fluid property  $\alpha$  is the mass density ( $\rho$ ) and k = 1,2,3 designates the x, y and z components (see Currie, 1993). This implies the continuity equation:

$$\frac{\partial \rho}{\partial t} + \frac{\partial}{\partial x_k} (\rho V_k) = 0 \tag{4.9}$$

This is more commonly written as:

$$\frac{\partial \rho}{\partial t} + \nabla \cdot \left( \rho \,\overline{V} \right) = 0 \tag{4.10}$$

Where  $\nabla$  is the del operator,  $\nabla = \frac{\partial}{\partial x}\hat{i} + \frac{\partial}{\partial y}\hat{j} + \frac{\partial}{\partial z}\hat{k}$  and u, v and w are the x, y and z components of the velocity  $\overline{V}$  respectively. This thesis assumes incompressible flow, in which case equation (4.9) reduces to

 $\nabla \cdot \overline{V} = 0 \tag{4.11}$ 

# 4.1.2 The Momentum Equation

The conservation of momentum equation applied to a system of fluid particle is conveniently treated as the Newton's second law of motion divided by the volume of the particle to deal with density rather than mass (White, 1991; Currie, 1993). The Cauchy equation e.g. Reddy (1998) is a more rigorous statement of the physical processes involved. This approach accounts for the external forces, which may act on the entire mass of the fluid, are body forces (i.e. gravitational or electromagnetic) or surface forces (pressure or viscous stresses). White (1991) expresses this relationship as follows.

$$\rho \frac{D\overline{V}}{Dt} = \overline{f} = \overline{f}_{body} + \overline{f}_{surface}$$
(4.12)

Considering gravitation as the only body force on the unit volume basis, gives

$$\overline{f}_{body} = \rho g \tag{4.13}$$

The surface forces are applied by external stresses on the sides of the element (see White, 1991) for the diagram. The stress describes the internal forces in the body; the product  $\tau \cdot \hat{n}$  gives the force per unit area acting on a surface in the body with the outward unit normal  $\hat{n}$ . This is a vector with components  $\tau_i = \tau_y \cdot \hat{n}_j$  (Reddy, 1998). The stress tensor  $\tau_y$  for the surface stresses can then be written as:

$$\tau_{ij} = \begin{pmatrix} \tau_{xx} \tau_{xy} \tau_{xz} \\ \tau_{yx} \tau_{yy} \tau_{yz} \\ \tau_{xx} \tau_{zy} \tau_{zz} \end{pmatrix}$$
(4.14)

For Newtonian fluids, FLOTRAN relates the stress and the rate of deformation of the fluid (in indicial notation) as follows:



$$\tau_{ij} = -p\delta_{ij} + \mu \left(\frac{\partial V_i}{\partial x_j} + \frac{\partial V_j}{\partial x_i}\right) + \delta_{ij}\lambda \frac{\partial V_i}{\partial x_i}$$
(4.15)

The equation (4.15) is called the constitutive relation (Currie, 1993). Balance of the angular momentum leads to symmetry of the stresses,  $\tau_{ij}$  forms a symmetric tensor, that is  $\tau_{ij} = \tau_{ij}$ . The symmetry satisfies equilibrium moments about the three axes of the element. The total surfaces forces in vector form is expressed as

$$\overline{f}_{surface} = \nabla \cdot \tau_{ij} = \frac{\partial \tau_{ij}}{\partial x_{j}}$$
(4.16)

Newton's law now becomes,

$$\rho \frac{DV}{Dt} = \rho \overline{g} + \nabla \cdot \tau_{ij} \tag{4.17}$$

"The divergence of  $\tau_{ij}$  should be interpreted as a tensor, so that result is a vector" (White, 1991). The stress tensor term  $\tau_{ij}$  may be expressed in terms of the velocity  $\overline{V}$  by relating the  $\tau_{ij}$  to the strain rate  $\epsilon_{ij}$  of viscous deformation (see White, 1991) for details. This yields the Navier Stokes momentum equation

$$\rho \frac{D\overline{V}}{Dt} = \rho \overline{g} - \nabla P + \frac{\partial}{\partial x_j} \left[ \mu \left( \frac{\partial V_i}{\partial x_j} + \frac{\partial V_j}{\partial x_i} \right) + \delta_{ij} \nabla \cdot \overline{V} \right]$$
(4.18)

For incompressible flow, equation (4.18) reduces to:

$$\rho \frac{D\overline{V}}{Dt} = \rho \overline{g} - \nabla P + \frac{\partial}{\partial x_j} \left[ \mu \left( \frac{\partial V_i}{\partial x_j} + \frac{\partial V_j}{\partial x_i} \right) \right]$$
(4.19)

in which the viscosity  $\mu$  may vary with temperature, pressure and position. Equation (4.19) is employed by FLOTRAN in this study. For constant viscosity, the momentum equation reduces to

$$\rho \frac{D\overline{V}}{Dt} = \rho \overline{g} - \nabla P + \mu \nabla^2 \overline{V} \quad . \tag{4.20}$$

# 4.1.3 The Energy Equation

This study outlines the basic steps that lead to this equation, (see White, 1991 for detail). The First Law of Thermodynamics may be written.

$$dE_t = dQ + dW \tag{4.21}$$

The quantity  $E_t$  includes both the internal energy, kinetic and the potential energy of the fluid particle, therefore the energy per unit volume is

$$E_{i} = \rho \left( e + \frac{1}{2} V^{2} - \overline{g} \cdot \overline{r} \right)$$
(4.22)

The time rate of change for equation (4.22)

$$\frac{DE_t}{Dt} = \rho \left( \frac{De}{Dt} + \overline{V} \frac{D\overline{V}}{Dt} - \overline{g} \cdot \overline{V} \right)$$
(4.23)

The transfer of heat Q through the fluid element is given by Fourier's law as

$$\overline{q} = -k\nabla T \tag{4.24}$$

The time rate of heat transfer neglecting internal heat generation is

$$\frac{DQ}{Dt} = -\nabla \cdot \overline{q} = +\nabla \cdot (k\nabla T)$$
(4.25)

The rate of work done to the element per unit area by the fluid entering the y-z plane or the left face (see page 70, White, 1991; for the diagram) is expressed as.

$$W_{x} = -\left(u\tau_{xx} + v\tau_{xy} + w\tau_{xz}\right) \tag{4.26}$$

Hence, for the y-z, y-x and z-x planes, that is the left, back and bottom sides is (using indicial notation) equation (4.26) is expressed as.

$$W = -\overline{V} \cdot \tau_{ij} \tag{4.27}$$

The net rate of work done on the element is

$$\frac{DW}{Dt} = -\nabla \cdot \overline{W} = \nabla \cdot (\overline{V} \cdot \tau_{ij})$$
(4.28)

This may be more conveniently expressed as.

$$\nabla \cdot \left( \overline{V} \cdot \tau_{ij} \right) = \overline{V} \cdot \left( \nabla \cdot \tau_{ij} \right) + \tau_{ij} \frac{\partial V_i}{\partial x_j}$$
(4.29)

The first term on the right hand-side is directly related to the momentum equation, which upon re- arrangement of terms yields the kinetic, and potential energy.

$$\overline{V} \cdot \nabla \tau_{ij} = \rho \left( \overline{V} \frac{D\overline{V}}{Dt} - \overline{g} \cdot \overline{V} \right)$$
(4.30)

The potential and kinetic terms vanish in equation (4.30) after  $E_t$ , Q and W from equations (4.23), (4.25), (4.28) are substituted into (4.21) to obtain the time rate of change first law of thermodynamics equation. This results in the first thermodynamic law for fluid motion (White, 1991).

$$\rho \frac{De}{Dt} = \nabla \cdot (k \nabla T) + \tau_{ij} \frac{\partial V_i}{\partial x_j}$$
(4.31)

The above energy equation can be transformed into the complete enthalpy equation using the stress tensor, which is then split into pressure and viscous terms below.

$$\tau_{ij}\frac{\partial V_i}{\partial x_j} = \tau'\frac{\partial V_i}{\partial x_j} - p\nabla \cdot \overline{V}$$
(4.32)

If the above equation and the continuity equation (4.11) are substituted, equation (4.31) becomes.

$$\rho \frac{D}{Dt} \left( e + \frac{p}{\rho} \right) = \frac{Dp}{Dt} + \nabla \cdot (k \nabla T) + \Phi$$
(4.33)

where fluid enthalpy is

$$h = e + \frac{p}{\rho} \tag{4.34}$$

The last term  $\Phi$  involves heating due to viscous stresses and is called the dissipation function.

$$\Phi = \tau_{ij} \frac{\partial V_i}{\partial x_j} \tag{4.35}$$

However, in this study the fluid enthalpy will be shelved for later, more advanced work as will be the viscous dissipation. The coefficient of thermal expansion  $\beta$  is useful in estimating the dependence of enthalpy on pressure.

$$dh = C_p dT + (1 - \beta T) \frac{dp}{\rho}$$
(4.36)

Equation (4.32) can be written into the energy equation to yield.

$$\rho C_{\rho} \frac{DT}{Dt} = \beta T \frac{Dp}{Dt} + \nabla \cdot (k \nabla T) + \Phi$$
(4.37)

The above equation can be alternatively expressed as.

$$\rho C_{p} \frac{\partial T}{\partial t} + \rho C_{p} (\overline{V} \cdot \nabla) T = \frac{\partial p}{\partial t} + (\overline{V} \cdot \nabla) p + k \nabla^{2} T + \Phi$$
(4.38)

Equation (4.37) is the energy equation for compressible flow. For incompressible flow the energy equation becomes.

$$\rho C_p \frac{\partial T}{\partial t} + \rho C_p (\overline{V} \cdot \nabla) T = k \nabla^2 T + \Phi$$
(4.39)

If there is a rationale for neglecting the viscous dissipation, then the energy equation for incompressible flow may be written as.

$$\rho C_{P} \frac{DT}{Dt} \approx k \nabla^{2} T \tag{4.40}$$

### 4.2 Buoyancy Driven Flows

Buoyancy forces drive magmatic fluids. Currie (1993) defines the buoyancy as the force experienced in a fluid because of variations of density in the presence of a gravitational field. Density variations are only important in the body force term of the Navier-Stokes equation, hence

•Compressibility is not of prime importance; only viscous effects are of primary importance.

•Buoyancy driven flow employs the Boussinesq approximation, which enables the use of the incompressible conservation equation to account for the buoyancy forces (Currie, 1993, Turcotte and Schubert, 1982).

For Pressure

$$p = p_0 + p^* \tag{4.41}$$

Density

$$\rho = \rho_0 + \rho^* \tag{4.42}$$

And Velocity

$$\overline{V} = \overline{V_0} + \overline{V}^* \tag{4.43}$$

Equations (4.41), (4.42) and (4.43) are then substituted into the continuity and the momentum equations (4.11) and (4.20) respectively, to obtain equations, which are applied to exact incompressible fluids, which have density variations or stratifications throughout (see page 312; Currie, 1993; Turcotte and Schubert, 1982). The Boussinesq approximation involves neglecting any other variation in density except those related to the gravitational term. Thus considering the density  $\rho$  constant, the Boussinesq approximation governing equations are:

The continuity equation:

$$\nabla \cdot \overline{V} = 0 \tag{4.44}$$

The momentum equation:

$$\rho \frac{\partial \overline{V}}{\partial t} + \rho (\overline{V} \cdot \nabla) \overline{V} = -\nabla p + \mu \nabla^2 \overline{V} - \Delta \rho g \overline{e}_z$$
(4.45)

 $\Delta \rho g \overline{e}_z$  is the buoyancy term and  $\overline{e}_z$  is the unit vector acting in the positive z direction. Gravity is assumed to act in the negative z direction.

### 4.2.1 Thermal Convection in magmas

Thermal convection is a natural heat transfer process, which occurs when the motion of the fluid is driven solely by density differences associated with temperature gradients.

Convection results from the emplacement of a body of fluid in an environment of higher or a lower temperature than that of the body. The temperature difference arising because of heat flow between the fluids causes a change in the density of the fluid in the vicinity of its surroundings or boundaries. This leads to a gravitational unstable situation because such density differences lead to a downward flow of the heavier fluid and the upward flow of the lighter fluid (Kreith and Bohn, 1993; Turcotte and Schubert, 1982; Currie, 1993). The relationship for the density variations with temperature is expressed as follows:

$$\Delta \rho = -\rho_0 \beta (T - T_0) \tag{4.46}$$

Equation (4.46) is valid only for moderate variations of temperature T from the reference value. However, a general representation for the equation of state (4.1) is expressed as follows after invoking the condition of incompressibility that.

$$\rho = \rho_o + (p - p_o) \frac{\partial \rho}{\partial p} (p_o, T_o) + (T - T_o) \frac{\partial \rho}{\partial T} (p_o, T_o)$$
(4.47)

This implies retaining only the linear terms of the pressure and temperature difference in a Taylor series expansion. Assuming negligible compressible effects, the second term on the right vanishes and density is expressed as a function of temperature only (Currie, 1993). Generally the property  $\beta$  is determined experimentally, except for ideal gases where  $\beta = \frac{1}{T_o}$ . After substituting equation (4.43) into the equation of motion, the Navier-Stokes equations for thermal convection may be written.

$$\nabla \cdot \overline{V} = 0 \tag{4.48}$$

$$\rho \frac{\partial \overline{V}}{\partial t} + \rho (\overline{V} \cdot \nabla) \overline{V} = -\nabla p + \mu \nabla^2 \overline{V} + \rho g \beta (T - T_o) \overline{e}_z$$
(4.49)

$$\rho C_{p} \frac{\partial T}{\partial t} + \rho C_{p} (\overline{V} \cdot \nabla) T = \frac{\partial p}{\partial t} + (\overline{V} \cdot \nabla) p + k \nabla^{2} T + \Phi$$
(4.50)

The buoyancy term couples the momentum equation (4.49) with the energy equation (4.50). Hence both must be employed together to obtain a closed mathematical system (Currie, 1993). Both equation (4.49) and (4.50) must be employed simultaneously, since both involve the parameters  $\overline{V}$  and T, since the velocity distribution is governed by the temperature distribution, but the temperature distribution depends upon the advection/convection of the heat and hence velocity distribution. Therefore, there is no possibility of determining one independent of the other (Tritton, 1977). The above information provides some of the reasons why free convection is hard to treat theoretically. Most of the information comes from experimental investigations.

### 4.2.1.1 Dynamic Similarity

With such experimental investigations one needs to know when dynamic similarity prevails. Since there is no velocity scale, which is provided on the specification of forced convection, one cannot define the Reynolds number using the parameters involved in setting up a problem. Also a temperature differences scale  $\theta$ , will only govern how vigorous the motion is. After treating equations (4.49) and (4.50) by using dynamic similarity, Tritton (1977) demonstrates that dynamic similarity depends on two non-dimensional parameters:

$$Gr = \frac{g\beta\theta d^3}{v^2}$$
(4.51)

 $\Pr = \frac{\nu}{\kappa} \tag{4.52}$ 

Equation (4.51) and (4.52) represent the Grashof and the Prandtl numbers respectively. The Prandtl number is the property of the fluid that restricts the transfer of information from one fluid, to the other; whereas the Grashof number, for any given fluid indicates the type of flow to be expected, that is, it indicates which dynamic processes are dominant, turbulent or laminar flow (Tritton, 1977). Physically, the Prandtl number is the ratio of momentum change due to viscosity to diffusion of heat due to conduction. The Grashof number is the ratio of the inertia forces to that of the viscous forces.

# • Orders of magnitude of inertia versus the buoyancy force

The inertia and buoyancy terms from equation (4.49), the momentum equation can be shown to yield the following approximation:

$$\overline{V} \cdot \nabla \overline{V} \approx \left| g \beta (T - T_0) \right| \qquad (4.53)$$

which leads to:

$$V^2/d \approx g\beta\theta$$
 (4.54)

Equation (4.53) yields the velocity scale to determine the rate at which the fluid flows as result of the temperature distributions, hence the approximate velocity magnitude.

$$V \approx \sqrt{g\beta d\theta} \tag{4.55}$$

# •Orders of magnitude of inertia and viscous forces

Comparing the inertia term with viscous terms, equation (4.49) now yields:

$$\frac{\left|\overline{V} \cdot \nabla \overline{V}\right|}{\left|\upsilon \nabla^2 \overline{V}\right|} \approx \frac{\rho V d}{\mu} \approx \left(\frac{g\beta d^3 \theta}{\upsilon^2}\right) = Gr^{\frac{1}{2}}$$
(4.56)

This relationship shows that, for large Grashof numbers, the viscous force is negligible compared with the buoyancy and the inertia forces. To deal with small Grashof numbers, Tritton (1977) compared the viscous force with the buoyancy force (see page 117 Tritton, 1977 for details). However, in solving free convection problems, one must know not only the important dynamic processes involved in determining the velocity distribution and its associated parameters, but also which other processes are relevant in determining the temperature distributions and related parameters. The relationship below was established when the advection and the conduction terms of equation (4.50), that is the energy, equation, were used:

$$\frac{Advection}{Conduction} \approx \frac{|\overline{V} \cdot \nabla T|}{|\kappa \nabla^2 T|} \approx \frac{\rho V d}{\mu}$$
(4.57)

Then for large Grashof numbers, the equation above becomes:

$$\left| \overline{V} \cdot \nabla T \right| \approx Gr^{\frac{1}{2}} \operatorname{Pr}$$
(4.58)

Equation (4.58) is valid only for small Prandtl numbers (as in liquid metals). However, for Large Prandtl numbers i.e., for viscous fluids, it is valid for oils and magmas. The relationship in (4.58) is represented by the quantity below:

$$Ra = Gr \Pr = \frac{g\beta d^3\theta}{\nu\kappa}$$
(4.59)

In equation (4.59), the Rayleigh number plays a crucial role in studies of horizontal layers. The Rayleigh number in equation (4.59) can be expressed in a form which expresses clearly the physical parameters involved,

$$Ra = \frac{\rho^2 g \beta d^3 C_p \theta}{\mu k} \tag{4.60}$$

The Rayleigh number is a function of the ratio of heat transfer by convection to that by conduction. During the cooling of the magma chamber, the Rayleigh number of the chamber decreases. This means that the heat transfer by conduction will eventually override that by convection (Rice, 1981). This decrease is due to the following.

• During cooling of magma, the country rock heats up as the magma cools. Therefore the temperature difference  $\theta$  decreases, causing Ra to decrease.

• Upon cooling the viscosity increases and therefore lowers the Rayleigh number.

• Magma solidification first starts to occur along the limbs (the cooler sides) decreasing the depth of the chamber. Convection thereafter decreases because the Rayleigh number is directly proportional to  $d^3$ . The Rayleigh number, (for a parallel plate of infinite horizontal extent and heated from below) has the following flow regimes (Khrishnamurti, 1970):

- If Ra≤ 1700, no convection occurs
- If  $1700 \le \text{Ra} \le 3 \ge 10^6$  the flow is laminar
- If  $Ra \ge 3x10^6$  the flow is turbulent

The Rayleigh number is a useful parameter in characterizing the type flow profiles of magma chambers

# 4. 3 Boundary layer thickness

The wall boundary layer is defined as the region near the wall where the convective velocities decrease to zero from mainstream values. This decrease in velocity is caused by viscous shear stresses at the wall. The distance from the wall at which the velocity reaches at least 99% of free stream velocity is called the boundary layer thickness (Kreith and Bohn, 1993). Flow adjacent the wall is completely laminar. However, at a critical distance from the wall, the inertial stresses come to a point where they override the viscous stresses and small perturbations start to develop. A transition from laminar to turbulent flow occurs when these perturbations are amplified (Kreith and Bohn, 1993). Clearly from the definition of viscosity in equation (3.9) shear stresses are the largest within the boundary layer of the magma. Therefore the importance of the boundary thickness cannot be dismissed. Rice and von Gruenewaldt (1995) emphasized that scavenging occurs in the boundary layer and hence the boundary layer may collect PGEs. The boundary layer thickness  $\delta$  of magma can be estimated using the following method; Newton's law of cooling may be employed to estimate convective energy flow.

$$q = h\Delta T \tag{4.61}$$

Here q is the heat transferred through the system per unit time per unit area,  $\Delta T$  is the temperature difference between the wall and the bulk temperature of the fluid and h is the film coefficient given by.

$$h = \frac{kNu}{d} \tag{4.62}$$

The Nusselt number (Nu) which can expressed as a function of the Rayleigh number.

$$Nu = AR^n \tag{4.63}$$

where A and n are experimentally determined constants. For turbulent flow, A = 0.13 and n = 1/3 (see Kreith and Bohn, 1993; Tritton, 1977; Turcotte and Schubert, 1982). Hence,

$$Nu = 0.13Ra^{1/3} \tag{4.64}$$

Tritton (1977) expressed the Nusselt number in terms of the boundary layer thickness

$$Nu = \frac{d}{\delta} \tag{4.65}$$

Equation (4.65) can be used to approximate the boundary layer thickness which is found to be.

$$\delta \approx 7.7 dRa^{-1/3} \tag{4.66}$$

This relationship provides a useful check when performing finite element analyses of fluid flow.

#### 4.4 Incompressible Turbulence:

The Rayleigh number calculations for magma chamber models used in this study are shown in table 4.1. These calculations give Rayleigh numbers above  $10^6$  for all the magma models used in this study. Using the turbulence criterion for flow between parallel plates (Krishnamurti, 1970; also see section 4.2.1.1), the Rayleigh number calculations in table 4.1 provide good rationale for invoking turbulence calculations.

Magma Models (M)	Depth (d) in (m)	Rayleigh Numbers (Ra)	Ra <sup>-1</sup> /3	Boundary Layer Approx $(\delta)$
M1 .	220	2.3X10 <sup>12</sup>	7.6X10 <sup>-5</sup>	0.129m
M2	450	2.0X10 <sup>13</sup>	3.7X10 <sup>-5</sup>	0.128m
M3	650	5.9X10 <sup>13</sup>	2.6X10 <sup>-5</sup>	0.130m
M4	950	1.84X10 <sup>14</sup>	1.8X10 <sup>-5</sup>	0.132m

**Table 4.1:** Rayleigh number and boundary layer approximations calculations for the magma models used in this study.

Turbulence is initiated when the inertial terms in the momentum equations greatly dominate the viscous terms in equation (4.49). Hence the instantaneous velocity of the fluid fluctuates at every point in the flow field. It is therefore convenient to express in terms of the mean value and a fluctuating component:

$$V_x = \left\langle V_x \right\rangle + V_x^* \tag{4.67}$$

Most of the research on turbulent flow analysis in the past century used the concept of time averaging (White, 1991). Applying the time averaging to the basic equations of motion yields the Reynolds equations, which involve both mean and fluctuating quantities (White, 1991). The time average for the fluctuating component is zero, that is

 $\frac{1}{\delta_{i}}\int_{0}^{\delta_{i}}V_{x}^{*}dt = 0; \text{ and for the instantaneous value is the average value: } \frac{1}{\delta_{i}}\int_{0}^{\delta_{i}}V_{x}dt = \langle V_{x} \rangle.$ 

Equation (4.67) is then substituted into the momentum equations, the time averaging leading to additional terms (see Ansys Flotran Theory Reference Manual (1977) for details). These additional terms when substituted into equation (4.20) and then after time averaging yields.

$$\rho \frac{D\overline{V}}{Dt} + \rho \frac{\partial}{\partial x_j} \left( \overline{V_i^* V_j^*} \right) = \rho \overline{g} - \nabla \overline{p} + \mu \nabla^2 \overline{V}$$
(4.68)

Equation (4.68) is the mean momentum equation it contains a new term involving the turbulent inertia tensor  $\overline{V_i V_j}$ , this term is never negligible in any turbulent flow and it is the source of analytic difficulties, because not much is known about its prior analytic form (White, 1991). The components of  $\overline{V_i^* V_j^*}$  are related not only to fluid physical properties but also to the local flow conditions (velocity, geometry, surface roughness and upstream history), but there are no further physical laws available to solve this dilemma (White, 1991). However, some of the successful empirical approaches with narrow formulation from non-rigorous postulates shed some light on equation (4.68), if it is rearranged to display the turbulent inertia terms as if they were stresses, which they are not. Hence (4.68) is.

$$\rho \frac{D\overline{V}}{Dt} = \rho \overline{g} - \nabla \overline{p} + \nabla . \tau_{ij}$$
(4.69)

where  $\tau_{ij} = \mu \left( \frac{\partial V_i}{\partial x_j} + \frac{\partial V_j}{\partial x_i} \right) - \left( \frac{\rho V_i^* V_j^*}{\omega r bulent} \right)$ , mathematically, the turbulent inertia terms act as

if the total stress on the system were composed of the Newtonian viscous stresses plus the additional stress tensor  $-\langle \rho V_i^* V_j^* \rangle$ . Much about the turbulent stresses is still unknown and the information that has been gained thus far is conceptual (White, 1991). The turbulent stress tensor above, also known as the Reynolds stress term, is generally expressed in the form (Ansys Flotran Theory Reference Manual, 1977).

$$\sigma^{R} = -\left\langle \rho V_{x} V_{y} \right\rangle \tag{4.70}$$

The Reynolds stress arises from the correlation of two components of the velocity fluctuations at the same point. A non-zero value of this correlation implies that the two components are not independent of one another, for example, if  $V_x V_y$  is negative, then

moments at which  $V_x$  is positive,  $V_y$  are more likely to be negative than positive, and *visa* -*versa* when  $V_x$  is negative. When transferred to co-ordinates at 45<sup>°</sup> to the x and y direction, this now correspond to anisotropy of the turbulence. Which means, different intensities in different directions (Tritton, 1977). Using

$$V'_{x} = \frac{\left(V_{x} + V_{y}\right)}{\sqrt{2}}$$

$$(4.71)$$

And

$$V_{y}' = \frac{\left(V_{x} - V_{y}\right)}{\sqrt{2}}$$

$$(4.72)$$

Yields

$$\left\langle V_{x}V_{y}\right\rangle = \frac{1}{2}\left(\left\langle V_{x}^{*2} - V_{y}^{*2}\right\rangle\right)$$
(4.73)

These equations demonstrate how such correlation arises in mean shear (see Page 246 Tritton (1977) for details). The equation for energy of the mean flow contains a term with opposite sign; such a term represents transfer of energy from the mean flow to turbulence (see page 247 Tritton, 1977). The Reynolds stress is such a term, in that it removes energy from the mean flow by providing that energy for turbulence (Tritton, 1977). This removed energy finally dissipates as heat because of the effect of viscosity on the turbulent fluctuations. This loss of mean flow energy to turbulence is large compared with the direct viscous dissipation (Tritton, 1977). Attempts have been made to relate the Reynolds stress to the mean flow in such a way that will allow the mean flow development to be calculated without the detailed study of turbulence. An example of such a procedure is the concept of eddy viscosity (Tritton, 1977). If we use the eddy viscosity approach to turbulence modeling, these terms are then put into the form of viscous stress term with the turbulent viscosity as the unknown coefficient, for example

$$-\left\langle \rho V_x V_y \right\rangle = \mu_t \frac{\partial V_x}{\partial y} \tag{4.74}$$

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This strategy is advantageous because the Reynolds stress terms are exactly the same as diffusion terms in the original Navier- Stokes equations. These two terms are then combined when the effective viscosity is defined as the sum of the laminar and turbulent viscosity, as shown in the following expression (White, 1991; Ansys Theory Reference manual, 1977).

$$\mu_{eff} = \mu_l + \mu_l \tag{4.75}$$

The solution of the turbulence model is based upon the solution of the eddy viscosity. The eddy viscosity has the same dimensions as  $\mu_1$ , the laminar viscosity but it is not a fluid property. It depends on the flow conditions and the geometry (White, 1991). The eddy viscosity is modelled with the following expression (White, 1991 and Ansys Theory Reference Manual, 1977).

$$\mu_{t} = C_{\mu}\rho \frac{E_{K}^{2}}{\epsilon}$$
(4.76)

where  $C_{\mu}$  is an empirical constant with the following experimental determined recommended values for attached boundary layer calculations,  $C_{\mu} = 0.09$  (White, 1991; Flotran Ansys Theory Reference Manual, 1977). This value is modified for other problems such as jets, wakes and recirculation (White, 1991). The solution to the Navier-Stokes turbulence equations is used to calculate the effective viscosity and effective thermal conductivity, using the following expressions.

$$\mu_{eff} = \mu + C_{\mu} \rho \frac{E_{\kappa}^{2}}{\varepsilon}$$
(4.77)

$$k_{eff} = k + \frac{\mu_t C_p}{\sigma_t} \tag{4.78}$$

where  $k_{eff}$  is the effective thermal conductivity and  $\sigma_i$  is the turbulent Prandtl number. The turbulent Prandtl number relates the eddy diffusion of the kinetic energy  $E_k$  and the kinetic energy dissipation rate ( $\varepsilon$ ) to the moment eddy viscosity. For wall element conditions the Reynolds number expressed as  $R_T = \rho \frac{E_K^2}{\mu \epsilon}$ . The  $k - \varepsilon$  turbulence model is invalid near a no-slip boundary wall if  $R_T$  value is very large (Ansys Theory Reference Manual, 1977; White, 1991). For such situations, the "Law of the Wall" and the "Log-Law of the Wall" models are used to approximate the turbulent boundary layer velocity profile. These models also provide a way of determining approximate values for the wall shear stress if a value for the velocity parallel to the wall ( $V_{tan}$ ) at a particular distance from the wall is given (White, 1991; Ansys Theory Reference Manual, 1977). The "Log-Law of the Wall" for the turbulent sub layer is expressed as follows

$$\frac{\overline{V}_{\text{tan}}}{\sqrt{\frac{\tau_{w}}{\rho}}} = \frac{1}{\kappa_{w}} \left( \ln \frac{E\delta}{v} \sqrt{\frac{\tau_{w}}{\rho}} \right).$$
(4.79)

The Compflo, inc Flotran Theory Reference manual (1992) derives equation (4.78). These calculations lead to the following expression the near -wall shear stress equation

$$\tau_{w} = \mu_{w} \frac{\overline{V_{\text{tan}}}}{\delta} \,. \tag{4.80}$$

For the derivation of equation (4.64) see The Compflo, inc. Flotran Theory Reference Manual (1992). The near-wall viscosity equation is then calculated from the wall shear stress above as.

$$\mu_{w} = \delta \frac{\tau_{w}}{u_{\text{tan}}} \tag{4.81}$$

The wall element viscosity value calculated from equation (4.81) is larger than the laminar viscosity (Ansys Theory Reference Manual, 1977). However, the  $k - \varepsilon$  model is

used to determine the turbulent kinetic energy near-wall values, where these values are calculated when the turbulent near-wall energy dissipation rate near a solid boundary is given by:

$$\varepsilon_{mw} = \frac{C_{\mu}^{\frac{\gamma_4}{4}} E_{\kappa_{mv}}^{\frac{\gamma_4}{2}}}{\kappa_w \delta}$$
(4.82)

Equation (4.82) is the near-wall energy dissipation rate (Compflo, inc. Flotran Theory Reference Manual, 1992). Alternatively, it is possible to use a wall formulation based on the equality of turbulence production and dissipation. The wall treatment can then be invoked by creating such conditions, a condition which yields an expression for a wall parameter  $Y^+$  (White, 1991) such that

$$Y^{+} = \frac{\mu_{0}^{\frac{1}{4}}\rho E_{K_{ff}\psi}}{\mu_{eff}} .$$
 (4.83)

The wall element effective viscosity and thermal conductivity are based directly on the value of  $Y^+$ . For the laminar sub-layer it extends to  $Y_t^+$  hence For  $Y^+ < Y_t^+$ :

$$\mu_{\rm eff} = \mu \tag{4.84}$$

$$k_{eff} = k \tag{4.85}$$

For  $Y^+ \ge Y_t^+$  (see Ansys FLOTRAN Theory reference Manual, 1977) for other details about the expressions (4.77) and (4.78) of the effective viscosity and the effective thermal conductivity (Ansys Flotran Theory Reference Manual, 1977; White, 1991).

# 4.5 Shear Driven Aggregation

The shear driven aggregation process is a tendency to develop a concentration of suspended particles in the boundary layers. This results from the Bagnold effect or dispersive pressure  $P_{\nu}$  (Komar, 1972).

$$P_{\nu} = \alpha \Lambda^{\frac{2}{3}} \mu \left( \frac{dV}{dy} \right) \tag{4.86}$$

It is related to the volume concentration of solids in the flow by.

$$\Lambda = \frac{1}{\left(\frac{C_0}{C}\right)^{\frac{1}{3}} - 1}$$
(4.87)

The relationship for viscosity that is employed in the above is.

$$\mu_{eff} = \mu_0 (1 - \gamma C)^{-2.5} \tag{4.88}$$

(see chapter 3 for details). The terms for  $P_{\nu}$  indicate it to be a powerful self-reinforcing process which, through  $\Lambda$  and  $\mu$ , grows as it concentrates, by effectively locking material into the regions where  $du/dy \sim 0$  at the velocity peaks in the boundary layers. This yielded PGEs concentration profiles like those seen in the Bushveld complex

(Rice and von Gruenewaldt, 1994,1995). Rice and von Gruenewaldt (1994,1995) gave a brief theoretical description of this collision process. The collision frequency  $b_{ij}$  between particles with radius  $r_i$  and  $r_j$  at concentrations of  $n_i$  and  $n_j$  (that is, the number of particles per unit volume) is given as.

$$b_{ij} = \frac{4G}{3} (r_i + r_j)^3 n_i n_j \tag{4.89}$$

This relationship implies that scavenging (particulate collision) will occur where shear is greatest. Shear also occurs within eddies in turbulent flow but they are maximum in the boundary layers confining the flow. In fig. (3.3b) of chapter3, material is transported from the center of the convection cell to the boundary layers where most of shear and thus scavenging occurs. This boundary layer is the region where most of the PGEs partitioned into sulphide liquid droplets. This may be cast in terms of continuous distribution function N(V,t) where N(V,t)dV is the particle concentration in the volume range V to V + dV. The collision frequency  $b_{ij}$  between particles of radius  $r_i$  and  $r_j$  at concentrations  $N_1$  and  $N_2$  then becomes.

$$b_{V_1,V_2} = \left(\frac{3}{4}\right)^{\frac{V_3}{3}} \frac{4G}{3} \left(V_1^{\frac{V_3}{3}} + V_2^{\frac{V_3}{3}}\right) N(V_1) N(V_2) dV_1 dV_2$$
(4.90)

Which yields an equation for the rate of shear aggregation (see Rice and von Gruenewaldt, 1994, 1995 for details and references). That is

$$\frac{\partial N(V_1)}{\partial t} = \left(\frac{3}{4\pi}\right)^{\frac{1}{2}} \frac{2G}{3} \int_{0}^{\infty} N(V_2) N(V_2 - V_1) \left[V_2^{\frac{1}{2}} - \left(V_1 - V_2\right)^{\frac{1}{2}}\right] dV_2$$

$$- \left(\frac{3}{4\pi}\right)^{\frac{1}{2}} \frac{4G}{3} N(V_1) \int_{0}^{\infty} N(V_1) \left(V_1^{\frac{1}{2}} + V_2^{\frac{1}{2}}\right) dV_2$$
(4.91)

for the total particle concentration

$$N = \int_{0}^{\infty} n(V) dV \tag{4.92}$$

For particles of uniform size, hence equation (4.90) reduces to:

$$\frac{dN}{dt} = -\frac{4G\alpha\phi N}{\pi}$$
(4.93)

The solution of the above is then:

$$\ln\left(\frac{N}{N_0}\right) = -\frac{4\alpha G\phi t}{\pi} \tag{4.94}$$

where  $\phi$  is the volume fraction and  $\alpha$  is the probability that collision will yield an aggregation. The parameter t, the 'retention time', is the time taken to sweep the fluid clear of certain particulate material of a given concentration N (Rice and von Gruenewaldt, 1994, 1995). To estimate the volume fraction of PGEs in the melt, Rice and von Gruenewaldt (1995) assumed a density of  $17 \text{ gm/cm}^3$  for PGEs with a concentration of 20ppb. They found the volume fraction to be about 10-9. Rice and von Gruenewaldt (1994,1995) showed that the removal of particles to the boundary layers a of melt about 0.5km thick to ore-grade material (5000ppb) in a layer of the order of a 1m thick at convective boundaries can be accomplished in about 100000 years. These values are of the same order of magnitude as predicted by the solidification times of magma chambers. However, calculations showed that on initial emplacement, the heat outflow is greatest hence; the shear would be highest, during these first stages when the convective heat transfer was most vigorous. Therefore, half the concentration could have been secured in the order of 10000 years. These authors finally emphasized that, theoretically it is immaterial whether the PGE are present as particles or dissolved in magma. PGEs are in essence part of the melt volume and therefore within the shear environment of the boundary layer the sulphide droplets will be exposed to a high R factor. The work of this dissertation is to secure a feel for the effect of geometry on the location of regions of high shear, hence to location of economically interesting PGEs deposits. Computational fluid dynamics employing Finite Elements have been applied to accomplish this.

### **CHAPTER 5**

#### NUMERICAL METHODS

#### FINITE ELEMENT GOVERNING EQUATIONS FOR MAGMA FLUID FLOW

## **5.1 Introduction**

The finite element method is a valuable tool in the solution of many engineering problems. In problems with complex geometry it is often difficult, if not impossible to set up a mathematical model without major simplifying assumptions to obtain an analytic solution, which might, in any case, not be realistic. One must then resort to numerical methods to solve mathematical models. The numerical technique used in this work is the finite element method. Finite element methods possess flexibility for handling problems in which the boundaries are irregular or in which the medium is heterogeneous or anisotropic. Finite difference methods are much more difficult to apply to problems of great complexities (Wang and Anderson, 1982). These approximate methods provide a rationale for operating on the differential equations that make up the model to transform them into a set of algebraic equations (Wang and Anderson, 1982). For magma chambers of arbitrary shape no analytical solutions exist for conductive and convective heat transfer in the fluid, nor for surrounding country rock that may be of porous or non-porous media.

#### 5.2 The Physical problem

A general physical problem often involves an actual structure or structural component subjected to certain loads. The idealization of the physical problem requires certain assumptions that lead to differential equations governing the mathematical model. The mathematical models addressed here are complex enough to require the use of finite element methods. Since the finite element methods are numerical procedures, it is always necessary to assess the accuracy of the solution obtained through them. If the accuracy criteria are not met, the finite element solution needs to be repeated with more refined solution parameters (finer meshes) until the desired accuracy is attained. A suitable mathematical model requires that it be constructed to secure maximum accuracy of the solution. Interpreting the accuracy of the solution of a mathematical model can also give an increased understanding of the actual physical problem that needs to be modeled. Also, more refined mathematical models can be chosen to increase insight into the physics and to assist in deciding which changes in the physical problem are necessary to provide more meaningful results (Bathe, 1996). A flow chart of the processes involved is provided in fig (5.1).

# 5.3 The Boundary Value Problem (BVP)

The boundary value problems (BVP's) are suitable prerequisites to the study of timedependent problems, and are ideal to introduce and motivate the finite element methods (Reddy, 1998). The general approach in solving *boundary value problems* (BVP) is to specify the problem domain  $\Omega$  of interest first. Then formulate the problem by specifying the unknown functions and some of its derivatives (if any) on the boundary  $\Gamma$ and the initial time t = 0 (Reddy, 1998). There are several approaches in finite elements to solve the boundary value problem. That of "weighted residuals" will be employed in discussions here.

#### 5.4 The Weighted Residuals Method

The governing differential equations and the boundary conditions of an arbitrary physical problem are expressed as (Cook, Malkus and Plesha, 1989; Reddy, 1998).

$$D\phi - f = 0$$
 in domain  $\Omega$  (5.1a)

$$B\phi - g = 0$$
 on boundary  $\Gamma$  (5.1b)

Generally, equation (5.1) is difficult to solve for the exact solution  $\phi = \phi(x, y)$ , hence the approximate solution  $\hat{\phi}$  is found. The approximate solution may be assumed to be a polynomial  $\hat{\phi} = \hat{\phi}(a, x, y)$  that satisfies the essential boundary conditions and contains

undetermined coefficients  $a_1, a_2, ..., a_n$ . The approximate solution is obtained when the values of the coefficients  $a_i$  are determined. The difference between the exact  $\phi$  and the approximate  $\hat{\phi}$  solution should be reasonably small (Cook, Malkus and Plesha, 1989). The difference between the exact solutions and the assumed solution can be expressed as residuals  $R_{\Omega}$  and  $R_{\Gamma}$  which are functions of x, y and  $a_i$ . That is,

$$R_{\Omega} = R_{\Omega}(a, x, y) = D\hat{\phi} - f \text{ (interior residual)}$$
(5.2a)

$$R_{\Gamma} = R_{\Gamma}(a, x, y) = B\hat{\phi} - g \text{ (boundary residual)}$$
(5.2b)

The residuals may vanish for some values of x and y but not all unless  $\hat{\phi}$  is the exact solution  $\hat{\phi} \cong \phi$ . Presumably,  $\hat{\phi}$  is a good approximation if the residual is small. Small residuals can be achieved by various schemes, each of which is designed to produce algebraic equations that can be solved for the *n* coefficients  $a_i$ . Some popular schemes are: Collocation, Least squares and the Galerkin approximation (see Cook, Malkus and Plesha, 1989; for details).

These approaches are analogous to variational principles used in physics to minimize some physical quantity over the problem domain; perhaps energy. Galerkin's method is described below.

#### 5.5 Galerkin's Method

The Galerkin method employs 'weight functions'  $W_i = W_i(x, y)$  to set the "weighted" averages of residual  $R_{\Omega}$  to zero (Cook, Malkus and Plesha, 1989). The mathematical expression is.

$$\int_{\Omega} W_i(x, y) R_{\Omega} dV = 0 \text{ for } i = 1, 2, ..., n \quad (5.3)$$

$$\int_{\Gamma} W_i R_{\Gamma} d\Gamma = 0 \tag{5.4}$$

This implies the residuals are taken to be orthogonal to the weight functions. The use Laplace's equation on  $\phi$  (equation 5.5 below) is a convenient example to demonstrate the application of Galerkin method to physical problems. That is,

$$\frac{\partial^2 \phi}{\partial x^2} + \frac{\partial^2 \phi}{\partial y^2} = 0 \tag{5.5}$$

where the unknown function  $\phi$  is defined throughout the problem domain ( $\Omega$ ) in a piecewise fashion. The function  $\phi$  will be defined in terms of its approximate value  $\hat{\phi}$  below.

# 5.6 The Approximate Solution

The approximate solution is represented as a series summation where each term is a product of the nodal value  $\hat{\phi}_L$  at the node associated with the nodal basis function  $N_L(x,y)$ , which is also called the interpolation function because it defines the trial solution throughout the problem domain. The basis functions  $N_L(x,y)$  will act as the weighting functions. The definition of node will follow.

By definition, the approximate solution  $\hat{\phi}$  is expressed as follows.

$$\hat{\phi} = \sum_{L=1}^{M} \hat{\phi}_L N_L(x, y)$$
 (5.6)

The trial solution  $\hat{\phi}$  is now applied to a region of the domain of the problem, this region defined as an "element". The element is taken small enough so that this approximation to the actual solution is considered sufficiently accurate. The term "finite element" arises from this context. The collection of elements, which contain a specific node L common to



all elements in the collection, forms a patch around L (the shaded area in fig 5.2). The nodal basis function  $N_L$  is zero along the boundaries of the patch and at all points exterior to it. It is equal to unity at the nodal point L. Similar patches are constructed over the entirety of the problem domain.

On substitution of the approximate solution, equation 5.6 into equation 5.1, the application of Galerkin's method then requires that.

$$\iint_{\Omega} \left( \frac{\partial^2 \hat{\phi}}{\partial x^2} + \frac{\partial^2 \hat{\phi}}{\partial y^2} \right) N_L(x, y) dx dy = 0$$
 (5.7)

The residual  $\left(\frac{\partial^2 \hat{\phi}}{\partial x^2} + \frac{\partial^2 \hat{\phi}}{\partial y^2}\right)$  is a measure of the extent to which the trial solution  $\hat{\phi}(x, y)$ 

will not satisfy Laplace's equation. The residual must be zero throughout the problem domain to satisfy Laplace's equation (Wang and Anderson, 1982). Galerkin's method secures the condition that the weighted average of the residuals is zero throughout the problem domain. Equation (5.7) leads to a system of M nodes algebraic equations to solve Laplace's equation approximately. The usefuness, hence the frequent use of Galerkin's method and the weighted residual method is evident in problems where variational principles do not exist for generating all governing equations. In such



Fig 5.2 The shape of linear interpolation function  $N_L(x,y)$ 

situations Galerkin's method or other weighted residual methods can be applied. The system of equations represented by equation (5.7), i.e., those generated by Galerkin's method, is the same as that of a system generated from a minimum dissipation principle (Wang and Anderson, 1982).

To reduce the order of the derivatives in the intergrand of equation (5.7) integration by parts is applied to equation (5.7) resulting into the generalized expression of the form.

$$\iint_{D} \left( \frac{\partial \hat{\phi}}{\partial x} \frac{\partial N_{L}}{\partial x} + \frac{\partial \hat{\phi}}{\partial y} \frac{\partial N_{L}}{\partial y} \right) dx dy + \int_{\Gamma} \left( \frac{\partial \hat{\phi}}{\partial x} n_{x} + \frac{\partial \hat{\phi}}{\partial y} n_{y} \right) N_{L} d\sigma = 0 \quad (5.8)$$

The second term on the right handside of equation (5.8) is proportional to the normal flux through the boundary weighted by N<sub>L</sub> on the boundary. It is important to note that if the influx on the boundary is zero, the boundary intergral term  $\int_{\Gamma} \left( \frac{\partial \hat{\phi}}{\partial x} n_x + \frac{\partial \hat{\phi}}{\partial y} n_y \right) N_L d\sigma = 0$  becomes zero. Then the intergrand on the left side of equation (5.8) only contains first derivatives, which then simplifies the problem significantly into the form.

$$\iint_{\Omega} \left( \frac{\partial \hat{\phi}}{\partial x} \frac{\partial N_L}{\partial x} + \frac{\partial \hat{\phi}}{\partial y} \frac{\partial N_L}{\partial y} \right) dx dy = 0 \quad (5.9)$$

The differential equations in equation 5.5 are defined as the 'strong' form of problem whereas the integral expressions above (e.g., equation 5.9) are defined as the "weak" form of the problem.

## 5.7 Implementation of the Finite Element Technique

The finite element technique is implemented with a variety of element types. However, because of simplicity and convenience only the triangular and rectangular elements are defined and discussed in the next sections. Thereafter, the finite element technique is finally implemented by the "element conductance method" which will be discussed later.

The latter method is more efficient in building up a system of equations sequentially from the algebraic equations presented in equation (5.7).

#### 5.7.1 Triangular elements

Each triangle element is defined by three nodes at its corners. The nodes are the points within the problem domain at which unknowns are computed. These unknown  $\phi_n$  are the values of the function  $\phi$  at the points (indicated by the subscript *n*) constituting the nodes. The nodal function  $\phi$  is defined within each element in terms of the nodal values by basis or interpolation functions over the problem domain. Consider the example of the finite element mesh shown in figure 5.4. The problem domain is divided into eighteen triangles and each triangle is given an element number and three node numbers with one node for each corner. The nodes are numbered consecutively and systematically and column by column. This systematic numbering of nodes is not a requirement but offers great help for memory storage needs. The archetypal triangular element (see figure 5.3) has node numbers i, j and m in a counterclockwise fashion where the coordinates are designated as  $(x_i, y_i), (x_j, y_j)$  and  $(x_m, y_m)$  and the unknowns at the nodes:  $\phi_i = \phi(x_i, y_i), \phi_j = \phi(x_j, y_j)$  and  $\phi_m = \phi(x_m, y_m)$ . The trial solution  $\hat{\phi}_L(x, y)$  defined in equation (5.6) is now applied throughout the triangular element by linearly interpolating the nodal values  $\phi_i, \phi_j$  and  $\phi_m$ .

This linear interpolation implies that with each triangular element e, the expression for the trial solution is:

$$\phi^{e}(x, y) = a_0 + a_1 x + a_2 y \tag{5.10}$$

The values of the undetermined coefficients in equation (5.10) can be determined by setting up these equations.

$$\phi_i = a_0 + a_1 x_i + a_2 y_i \tag{5.11}$$

$$\phi_j = a_0 + a_1 x_j + a_2 y_j \tag{5.12}$$

$$\phi_m = a_0 + a_1 x_m + a_2 y_m \tag{5.13}$$

Equations (5.11), (5.12) and (5.13) can be solved for  $a_0, a_1$  and  $a_2$  and substituted back into equation (5.10) with the resulting equation :

$$\hat{\phi}^{e}(x,y) = N_{i}^{e}(x,y)\phi_{i} + N_{i}^{e}(x,y)\phi_{i} + N_{m}^{e}(x,y)\phi_{m}$$
(5.14)

where

$$N_i^e(x,y) = \frac{1}{2A^e} \Big[ (x_j y_m - x_m y_j) + (y_j - y_m) x + (x_m - x_j) y \Big]$$
(5.15)

$$N_{j}^{e}(x,y) = \frac{1}{2A^{e}} \Big[ (x_{m}y_{i} - x_{j}y_{m}) + (y_{m} - y_{j})x + (x_{i} - x_{m})y \Big]$$
(5.16)

and



Figure 5.3: The Archetypal triangular element e. The nodes are labeled i, j and m in counter –clockwise order. This diagram is taken from Wang and Anderson (1982)

$$N_m^{\ e}(x,y) = \frac{1}{2A^e} \Big[ (x_i y_j - x_j y_i) + (y_i - y_j) x + (x_j - x_i) y \Big]$$
(5.17)

The area of the triangle  $A^{e}(ijm)$  in terms of its coordinates at the corners is expressed as follows:

$$2A^{e} = (x_{i}y_{j} - x_{j}y_{i}) + (x_{m}y_{i} - x_{i}y_{m}) + (x_{j}y_{m} - x_{m}y_{j})$$
(5.18)

The functions  $N_i^e(x, y), N_j^e(x, y)$  and  $N_m^e(x, y)$  are the element interpolation or basis functions. These basis functions are functions of spatial coordinates x and y; and they define  $\hat{\phi}(x, y)$  in the element e in terms of the nodal values  $\phi_i, \phi_j$  and  $\phi_m$ .

#### 5.7.2 The Rectangular Element

The use of a four node rectangular is very restrictive in accomodating irregular boundaries. To accommodate irregular boundaries the quadrilateral element is transformed to the more useful isoparametric quadrilateral element (see appendix C, Wang and Anderson, 1982). The application of the Galerkin Method to rectangular elements requires that a basis function be defined over each rectangle. The four corner nodes are points at which the functions  $\phi_L(t)$  are unknowns. The archetypal rectangle is orientated parallel to the coordinate axes with its center at the local origin and the corners of the rectangular element e are labelled in a counterclockwise order i, j, m and nbeginning with the lower left corner.

The trial solution  $\hat{\phi}^e(x, y, t)$  over the rectangular element is:

$$\hat{\phi}^{e}(x,y,t) = N_{i}^{e}(x,y)\phi_{i}(t) + N_{i}^{e}(x,y)\phi_{i}(t) + N_{m}^{e}(x,y)\phi_{m}(t) + N_{n}^{e}(x,y)\phi_{n}(t)$$
(5.19)

The four basis functions, called the bilinear interpolations functions, are represented as follows:

$$N_i^{e}(x,y) = \frac{1}{4} \left( 1 - \frac{x}{a} \right) \left( 1 - \frac{y}{b} \right)$$
(5.20)

$$N_{j}^{e}(x,y) = \frac{1}{4} \left( 1 + \frac{x}{a} \right) \left( 1 - \frac{y}{b} \right)$$
(5.21)

$$N_{m}^{e}(x,y) = \frac{1}{4} \left( 1 + \frac{x}{a} \right) \left( 1 + \frac{y}{b} \right)$$
(5.22)

$$N_n^{e}(x,y) = \frac{1}{4} \left( 1 - \frac{x}{a} \right) \left( 1 + \frac{y}{b} \right)$$
(5.23)

where

$$2a = x_{j} - x_{i} = x_{m} - x_{n}$$
(5.24)  
$$2b = y_{n} - y_{i} = y_{m} - y_{j}$$
(5.25)

Each basis function varies linearly with distance along any side and has the property that  $N_L^{e}(x, y)$  is 1 at node L and 0 at the other three nodes.

The element basis function now defined in terms of the time derivatives  $\frac{\partial \phi_L}{\partial t}$  at the nodes

and the spatial variation of  $\frac{\partial \hat{\phi}^e}{\partial t}$  over the element is as follows:

$$\frac{\partial \hat{\phi}^{e}}{\partial t} = N_{i}^{e}(x,y)\frac{\partial \phi_{i}}{\partial t} + N_{j}^{e}(x,y)\frac{\partial \phi_{j}}{\partial t} + N_{m}^{e}(x,y)\frac{\partial \phi_{m}}{\partial t} + N_{n}^{e}(x,y)\frac{\partial \phi_{n}}{\partial t}$$
(5.26)

The same interpolation is used for the time derivative of the trial solution (Wang and Anderson, 1982). The same definition can be applied for rectangle not centered at the



origin but whose sides are still parallel to the coordinate axes. If the limits of integration are between -a and +a, and between -b and +b, a translation to the origin of the coordinate axes does not affect the value of the integration over the rectangle.

# 5.7.3 The Conductance Matrix

A sequential system of equations from equation (5.7) is built up by proceeding through the problem domain sequentially element by element and incorporating the contributions of element *ijm* to the three rows of any node L = i, L = j, and L = m until the
contributions of the last element have been summed. The first of the derivatives of equation (5.8) contains derivatives of the element-by-element definition of the  $N_L$ 

It is convenient to return now to the use of results obtained by integration by parts equation (5.8) which makes it possible to write equation (5.7) as a summation of integrals over individual elements equal to a boundary integral.

$$\sum_{e} \left\{ \iint_{e} \left( \frac{\partial \hat{\phi}^{e}}{\partial x} \frac{\partial N_{L}}{\partial x} + \frac{\partial \hat{\phi}^{e}}{\partial y} \frac{\partial N_{L}}{\partial y} \right) dx dy \right\} = \iint_{e} \left( \frac{\partial \hat{\phi}}{\partial x} n_{x} + \frac{\partial \hat{\phi}}{\partial y} n_{y} \right) N_{L} d\sigma \quad (5.27)$$

The function  $\hat{\phi}$  has been replaced by  $\hat{\phi}^e$  which is the function on the element *e*. The equation which defines  $\hat{\phi}^e(x, y)$  shows that  $\frac{\partial \hat{\phi}^e}{\partial x}$  and  $\frac{\partial \hat{\phi}^e}{\partial y}$  can be written in terms of the nodal functions  $\phi_i, \phi_j$  and  $\phi_m$  and derivatives of the element basis function (See page 122, Wang and Anderson, 1982, for these expressions). When the derivatives of  $\frac{\partial \hat{\phi}^e}{\partial x}$  and  $\frac{\partial \hat{\phi}^e}{\partial x}$  are substituted back into equation (5.27), the result is:  $G_{L,1}\phi_1 + \ldots + G_{L,i}\phi_i + \ldots + G_{L,m}\phi_m + \ldots + G_{L,m}\phi_M = f_L$  (5.28)

Equation (5.28) represents a system of M node equations which can be represented in matrix form as.

$$[G]\{\phi\} = \{f\} \tag{5.29}$$

The element conductance matrix is set up by subdividing the problem domain into elements evaluating the left-handside of the integral equation (5.29) one element at a time. N<sub>L</sub> is defined in the element e about the patch L to be the basis function  $N_L^e$  where the element e made up of nodes i, j and m contributes only to three equations in which L = i, j and m and e contributes to only to terms in  $\phi_i, \phi_j$  and  $\phi_m$ .

To put it succinctly, element e contributes to three rows and three columns of the coefficient matrix [G], which produes a  $3 \times 3$  matrix

$$\begin{bmatrix} G^{e} \end{bmatrix} = \begin{pmatrix} G_{ii}^{e} & G_{ij}^{e} & G_{im}^{e} \\ G_{ji}^{e} & G_{jj}^{e} & G_{jm}^{e} \\ G_{mi}^{e} & G_{mj}^{e} & G_{mm}^{e} \end{pmatrix}$$
(5.30)

The individual terms in the element conductance matrix are found by evaluating the double integral over element e in equation (5.29) for the entries along row L. For their derivation see page 124, Wang and Anderson (1982). In summary, the expression for the Global conductance matrix is as follows:

$$G_{L,i} = \sum_{e} G_{L,i}^{e}$$
(5.31)

The Global conductance matrix is not assembled by using one row at a time. Instead the element contributions to the global coefficient matrix are sorted out by subscript pairs; L,i;L,j and L,m since the elements are sorted one at a time. Further details on the description of the sorting process, are found on page 125 Wang and Anderson (1982). The assembly of the global matrix is done strictly in terms of the geometry node and element labelling of the finite element mesh. The components of column vector  $\{f\}$  in equation (5.29) are given by the boundary integral in equation (5.27) one for each nodal basis NL. If L is the interior node and no side of an element in the patch about L is part of the boundary, then  $N_L = 0$  over the whole boundary. Since  $N_L$  is the weighting function of the boundary integral then the entire integral is zero for all interior nodes L, hence  $f_L = 0$  if the subscript L represents an interior node, regardless of the boundary conditions. For details on the treatment of handling of boundary conditions when L represents the a boundary node see pages 126, 127 and 128, Wang and Anderson (1982). The next section discusses a commercial code which employs similar procedures to do calculations on convective and conductive processes in Newtonian and non-Newtonian fluids.

#### 5.8 ANSYS 5.6

Ansys is a commercial code used extensively in a variety of engineering and multiphysics disciplines. Ansys can do analysis ranging from structural, thermal, Computational Fluid Dynamics (CFD) to electromagnetics. However, for this study, use is made of the CFD code known as FLOTRAN. FLOTRAN in Ansys uses the Galerkin Finite Element Method and the Streamline Upwind Method to solve the Navier- Stokes, the continuity and the energy equations. Upwind methods utilize upstream data to estimate downstream conditions which conforms to the natural sequence of events, as opposed to the methods which violate physical laws by propagating information upstream (e.g. Roache, 1972). The next sections give a brief description of how FLOTRAN applies the concepts discussed in the previous sections to perform calculations of fluid dynamical problems.

#### 5.8.1 Discretization of the Governing Equations

The fluid governing equations already discussed in section 4.1 all have the form of the generic scalar transport equation, equation (5.32). For the sake of describing the discretizing methods, the variable  $\phi$  is used. This variable can represent either the temperature or a velocity component. The general scalar transport equation is:

$$\frac{\partial}{\partial t} \left( \rho C_{\phi} \phi \right) + \nabla \cdot \left( \rho C_{\phi} \phi \overline{V} \right) = \nabla^2 \left( \Gamma_{\phi} \phi \right) + S_{\phi}$$
(5.32)

The transient term is solved using the finite difference technique, whereas the advection term is solved using the Monotone Streamline Upwind method (see Rice and Schnipke, 1985 for detail) and the diffusion and source terms on the right hand side are solved using the Galerkin Method. The Galerkin method can lead to small magnitude non-physical oscillations. These non-physical oscullations are eliminated by the Monotone Streamline Upwind Method (brief details about latter methods follow in section 5.8.3).

Equation	$\phi$	$C_{\phi}$	$\Gamma_{\phi}$	$S_{\phi}$
Navier-Stokes	V	1	μ	$-\nabla p + \rho \overline{g}$
Energy	T	C <sub>p</sub>	k <sub>m</sub>	$\frac{\partial p}{\partial t} + \overline{V} \cdot \nabla p + \Phi$
Continuity	1	1	0	

 Table 5.1 Shows the generic scalar transport equations for incompressible Newtonian fluids

The meaning of the symbols has already been explained in Chapter 4.

The discretisation essentially consist of deriving the element matrices assembled into the form:

$$\left(\left[A_{e}^{transient}\right] + \left[A_{e}^{advection}\right] + \left[A_{e}^{diffusion}\right]\right)\left\{\phi_{e}\right\} = \left\{S_{e}^{\phi}\right\}$$
(5.33)

The Galerkin method will be used to form element integrals, (see equation (5.27)). The weighting function for the element will be denoted by  $W^e$ . This is also called the shape function (Ansys Theory Reference Manual, Spencer et al, 1997).

#### 5.8.2 The Transient Term

In solving parts of the differential equations, steady-state (time-independent) problems are only addressed when the time-dependent (transient) solutions are very small, however, the transient (time-dependent) solutions are more convenient. The use of finite difference or the finite element techniques depend on the complexity of the problem domain and which method best describes the problem in the most simple, efficient and cost effective manner with regard to computational resources, for instance computer memory and time. Ansys uses both of these techniques. The transient analysis is preferred over a steady-state approach to solve flow problems since it gives an insight into the behaviour of the fluid flow at its initial stages before reaching a fully developed flow. The finite element technique used by Ansys for the transient term is shown in equation (5.34) below.

$$\left[A_{e}^{transient}\right] = \int W^{e} \frac{\partial (\rho C_{\phi} \phi)^{e}}{\partial t} dV$$
 (5.34)

Total mass is employed such that.

$$\int W^{e} \frac{\partial(\rho C_{\phi} \phi)}{\partial t} dV = \frac{\partial(\rho C_{\phi} \phi)}{\partial t} \int W^{e} dV$$
(5.35)

The transient term is then treated with a backward difference constructed by a discretization process which uses a Taylor Series expansion that is a function of internodal spacing. For example for an arbitrary time-step n and its immediate backward time-step n-1, the Taylor expansion for  $\Theta$  at time n is,

$$\Theta_{n} = \Theta_{n-1} + \frac{\partial \Theta}{\partial t} \bigg|_{n} \Delta t + \frac{1}{2} \frac{\partial^{2} \Theta}{\partial t^{2}} \bigg|_{n} \Delta t^{2} + \dots HOT$$
(5.36)

where  $\Theta = \rho \phi$  and  $\Delta t$  is the time interval between times n-1 and n and HOT are the Higher Order Terms. After neglecting higher order terms, equation (5.36) is represented as.

$$\frac{\partial \Theta}{\partial t}\Big|_{n} = \frac{\Theta_{n} - \Theta_{n-1}}{\Delta t} + O(\Delta t^{2})$$
(5.37)

The order of error is denoted by  $O(\Delta t^2)$ . Flotran uses three backward differences with time steps n-2, n-1 and n and the three time intervals associated with them leads to.

$$\frac{\partial(\rho\phi)}{\partial t}\Big|_{n} = \frac{(\rho\phi)_{n-2} - 4(\rho\phi)_{n-1} + 3(\rho\phi)_{n}}{2\Delta t} + O(\Delta t^{2})$$
(5.38)

The nth time step produces a contribution to the diagonal of the element matrix which assists convergence, while the derivatives from the previous time steps form contributions to the source term.

#### 5.8.3 The Advection Term

The Galerkin finite element method gives rise to central-difference type approximations of differential equations. This method when applied to most structure or heat conduction problem leads to symmetric stiffness matrices such that the solution ends up possessing the best approximation property; this minimizes the difference between the finite element and exact solution to a certain norm. However, a serious drawback of this method is encountered when it is applied to problems involving fluid flow or convective heat transfer. The matrix associated with the convective term is nonsymmetric and as such the best approximation is lost. There are some terms for which the Galerkin method produces spurious results in parts of the problem domains used (Rice and Schnipke, 1985). In practice these solutions are often corrupted with spurious node- to-node oscillations or 'wiggles'. The reason is that for high Reynolds or high Peclet numbers the downstream boundary condition forces a rapid change in the solution. The only way to eliminate these the oscillations is to do a severe mesh refinement such that the convection no longer dominates on an element level. Mesh refinement is needed in regions where accurate representation of the solution is required but if a global solution feature is desired mesh refinement is needed only to prevent oscillation. This provided motivation for the development of an alternative to the Galerkin formulation which overrides the spurious oscillations regardless of the mesh refinements. The Upwind differencing method for the convective term was developed to yield 'wiggle'-free solutions (Brooks and Hughes, 1982). The use of upwind approximations for the advection terms, to stabilize advectiondominated transport and flow problems has received much critical attention in recent literature (Brookes and Hughes, 1982). It essentially amounts to approximating the

convective derivatives with solution values at the upstream central nodes of a threenode-stencil; its drawback is that the upwind differences are only first order accurate whereas the central –difference is second order accurate. The loss of accuracy is shown in diffuse solutions. The problem of the diffuse solutions were addressed when the upwinded method was reconstructed by adding the artificial diffusion (or viscosity) to the central - difference treatment. The inclusion of the artificial diffusion in the upwind method generated severe criticism of the upwind method. For further details on artificial diffusion, see Brooks and Hughes (1982). Because of the impetus provided by the fact that upwind methods are the only means to secure stable solutions for intense flow, these criticisms have been addressed and the treatment of the upwinded convective terms have been developed in a variety of ways. For example:

• By modifying the weighted function to achieve the upwind effect: since the modified weigh function is applied to all terms in the equations, the upstream node is weighted more heavily than the downstream of a node. This method is consistent with Petrov-Galerkin method of weighted residuals.

• By the Optimal 'smart' Upwind method: this was developed by Hughes from the Variational principle, which demonstrated the upwind method may be derived from a firm theoretical basis. This method leads to a system of matrix equations that give exact solutions for 1-D problems, but when generalized to more complicated, multi-dimensional problems, it leads to excessive diffusion perpendicular to the flow direction.

However, overly diffuse results also appear in transient problems, or when source terms are present. Recent developments have shown that when the upwind method is constructed with the Petrov-Galerkin weighted residual formulation none of the above problems are encountered (Brooks and Hughes, 1982). All of the above problems are eliminated when the Streamline Upwind /Petrov-Galerkin formulation is used which has the robustness of a classical upwind method. Furthermore it is not constrained by any of the artificial diffusion problems described above, since the upwind method adds diffusion or viscosity that acts only in the flow direction. If extended to the Petrov-Galerkin formulation, the standard Galerkin weighting function is modified by adding a streamline of upwind perturbation which acts only in the flow direction and the modified weighted function is then applied to all terms in the equation resulting in a consistent residual formulation. For more details see Brooks and Hughes (1982). The Monotone Streamline Upwind method is used by FLOTRAN to solve the Navier–Stokes advection term. This method, a detailed description of which appears in Rice and Schnipke (1985), is summarized as follows. It basically approximates first order derivatives by advection transport where it is assumed that there is no transfer across characteristic streamlines: all the transfer occurs along the streamlines with no physical diffusion (pure advection). The Monotone Streamline Upwind approach represents a direct streamline upwind approximation rather than modifying the weighting functions as is the case with the previously outlined methods, with the result that it treats test cases without the generation of non-physical spatial oscillations.

For a 3-D steady state flow dominated by advection, this approach can be described as follows: when the equation below

$$\frac{\partial(\rho V_x \phi)}{\partial x} + \frac{\partial(\rho V_y \phi)}{\partial y} + \frac{\partial(\rho V_z \phi)}{\partial z} = 0$$
(5.39)

is written in terms of the streamline distance s, the streamline coordinated system becomes one dimensional and hence is expressed as follows:

$$\frac{d(\rho V_s \phi)}{ds} = 0 \tag{5.40}$$

The above equation (5.40) was the basis for the streamline approximation used in the work of Rice and Schnipke (1985). The above equation indicates that, in the absence of other effects such as diffusion or source terms, the value  $\phi$  is constant along the streamline. The streamline equation (5.40) is assumed constant on an element

$$\frac{d(\rho V_s \phi)}{ds} = \text{constant}$$
(5.41)

Hence, with this assumption, Rice and Schnipke (1985) were able to evaluate the contribution of the advection term to the element matrix directly. The element advection term was then expressed as follows:

$$\left[A_e^{advection}\right] = \frac{d(\rho V_s \phi)}{ds} \int W^e dV$$
(5.42)

This formulation is made for every element, each of which will have only one node which receives contributions from the element. The gradient can be calculated using a simple difference formula:

$$\frac{d(\rho V_s \phi)}{ds} = \frac{(\rho V_s \phi)_U - (\rho V_s \phi)_D}{\Delta s}$$
(5.43)

where D is the subscript for value at the downstream node, U is subscript value taken at the location at which the streamline through the downwind node enters the element and  $\Delta s$  is the distance from the upstream point to the downstream node. The value at the upstream location is unknown but can be expressed in terms of the unknown nodal values that it lies between. The figure 5.5 demonstrates the Streamline Upwind Approach along the streamline. This process consists of cycling through all the elements and identifying the downwind nodes. A calculation is made based on the velocities to determine the direction the streamline exited upwind node. Weighting factors are also calculated based on the proximity of the upwind location to the neighbouring nodes.

#### 5.8.4 The Diffusion term

The expression for the diffusion terms comes from integration over the problem domain with the weighting function. The diffusion contribution is then

$$\begin{bmatrix} A_e^{diffusion} \end{bmatrix} = \frac{\int W^e \frac{\partial}{\partial x} \left( \Gamma_{\phi} \frac{\partial \phi}{\partial x} \right) dV + \int W^e \frac{\partial}{\partial y} \left( \Gamma_{\phi} \frac{\partial \phi}{\partial y} \right) dV}{+ \int W^e \frac{\partial}{\partial z} \left( \Gamma_{\phi} \frac{\partial \phi}{\partial z} \right) dV}$$
(5.44)

The x, y and z terms all treated in the same manner. After integrating the x-direction terms by parts, the outcome is.

$$\int W^{e} \frac{\partial}{\partial x} \left( \Gamma_{\phi} \frac{\partial \phi}{\partial x} \right) dV = \int \frac{\partial W^{e}}{\partial x} \Gamma_{\phi} \frac{\partial \phi}{\partial x} dV$$
(5.45)

Then the derivative of  $\phi$  is replaced by the nodal values and the derivatives of the weight function  $\phi$ .



Figure 5.5: Streamline Upwind Approach. This Diagram is taken from the Ansys Flotran Theory Reference Manual

The term 'downwind' defines a node for which the negative velocity vector at the node points back into the element. See Rice and Schnipke for more details (1985)

$$\frac{\partial \phi}{\partial x} = W_x^e \phi \tag{5.46}$$

$$\frac{\partial W^e}{\partial x} = W_x^e \tag{5.47}$$

The diffusion matrix may then be expressed as follows:

$$\left[A_{e}^{diffusion}\right] = \int \sum_{k=1}^{3} W_{k}^{e} \Gamma_{\phi} W_{k}^{e} dV$$
(5.48)

#### 5.8.5 The Source terms

The evaluation of the source terms is accomplished by multiplying the source terms by the weighting function and as shown by figure 5.5, then integrating over the volume.

$$S_{\phi}^{e} = W^{e}S_{\phi}dV \tag{5.49}$$

#### 5.9 Segregated Solution Algorithm

This solution algorithm is a process used by FLOTRAN to solve each degree of freedom such as temperature, pressure and the velocity components. The energy and the continuity equations are solved sequentially (see, Ansys Flotran Theory Manual, 1977; for details on the procedures leading to formation of the coupling equations ). These equations are coupled such that each degree of freedom is solved with the intermediate of the other degree of freedom. The process of solving all these equations and then updating the fluid properties is called a global iteration. See the Flow Chart in Figure 5.6, which shows a detailed summary of the steps involved.

#### 5.10 Solution Methods

In most field applications, a flexible model which allows consideration of an anisotropic and an heterogeneous medium is desired. There are adequate iterative techniques for solving simple problems but more complex models are best solved through the use of a combination of direct methods and iteration. Direct methods solve a system of linear algebraic equations by using only a sequence of operations whereas the iterative methods write and solve a generalized expression repetitively for every node in the problem domain. A combination of both is necessary (Wang and Anderson, 1982). These algorithms require repeated solutions to the matrix equations during global iterations, because in some cases an exact solution must be obtained, while in others approximate solutions are adequate and in certain cases the equations need not be solved at all. It has also been found that for the momentum equations, the time saved by calculating approximate solutions offsets the slightly slower convergence rates one obtains with an exact solution whereas for the pressure equation, exact solutions are required to ensure that the principle of mass conservation is maintained. For thermal problems with constant properties, there is no need to solve the energy equation at all until the flow problem has converged. Therefore, to accommodate these diverse requirements, FLOTRAN use two types of solvers, and both of them are iterative. The first is the sweeping method known as the Tri-Diagonal Matrix Algorithm (TDMA) and the second one is the Semi-Direct solver known as the Conjugate Direction Method. The user has control over which method to use for a degree of freedom.

#### 5.10.1 Tri – Diagonal Matrix Algorithm (TDMA)

This method consists of breaking down the problem domain into a series of tri-diagonal elements where the entries outside the tri-diagonal are treated as source terms using the previous values. The latter technique is named the Thomas Algorithm and is explained briefly in page 96 of Wang and Anderson (1982).

A detailed explanation of the TDMA is given by Patankar (1980). However for a completely unstructured mesh or an arbitrarily numbered system, the method reduces to the Gauss-Seidel iterative method. Since it is an approximate method, the TDMA is repeatedly executed until it satisfies a user defined convergence criterion. For the calculations done in this research use has been made of the TDMA method.

#### 5.10.2 The Conjugate Direction Method

This method is a combination of Conjugate Gradient and Conjugate Residual systems, where the first is for symmetric systems and the latter for non-symmetric systems. Iterative methods are used to attempt a solution to the equation of interest, where an incompressible flow is used for the pressure equation. The method develops a solution as a linear combination of orthogonal vectors. These vectors are generated one at a time during an iteration. In the Conjugate Gradient Method, the symmetry of the coefficient

matrix and the process of generating vectors ensures that each one is automatically orthogonal to all the previous vectors (Ansys Flotran Theory Reference Manual, 1977). In this method unlike with the TDMA, a convergence criterion and a maximum number iteration are specified by the user. The conjugate methods was not used in this work's calculations.



#### **CHAPTER 6**

### MAGMA AND COUNTRY-ROCK MODELS OF THE GREAT DYKE, ZIMBABWE

#### Introduction:

This thesis models a magma chamber and country rock intrusive system with a particular attention to the Great Dyke configurations. The work discussed in the previous sections provided and developed a clear and firm insight into the understanding of the theoretical and experimental foundation needed by the author to engage in this kind of research. This knowledge accumulated from understanding the background theory of fluids, their behaviour and the various processes involved in magmas, made it possible to construct and model both transient laminar and turbulent flows in magma chambers. The physical properties of magmas used in section 3 to plot curves in figures 3.4 and 3.5, were taken from experimental data derived from already cited literature. However, at this stage a closer look will be made at the values of the coefficients calculated using the curve-fit formula, the boundary conditions, initial conditions and the actual structure of the models used in this study.

#### 6.1 Magma and Country Rock physical properties

This section in table 6.1 lists only the values used for modeling Colombia River Basalts (CRB) because the magma fluid properties were already discussed in the previous sections. The country rock model is treated as a solid and non-porous medium with constant physical properties. These physical properties were derived from those of continental crusts with depth thickness varying from 0-30 km (see Bott, 1982). The models used simulate a magma chamber without a country rock and a magma-country rock intrusive system with the magma chamber completely surrounded by the country rock. The values for the physical properties of the country rock are listed in table 6.2

Fluid Property	Coefficient	Value
1. Viscosity	Nominal Viscosity $(\mu_0)$ Nominal Temperature $(T_0)$ Linear Coefficient $(a_1)$ Quadratic Coefficient $(a_2)$	15848.932 (Pas) 1473 (K) 35354.589 (K <sup>-1</sup> ) 32863277.255 (K <sup>-1</sup> ) <sup>2</sup>
2. Density	Nominal Density ( $\rho_0$ )Nominal Temperature ( $T_0$ )Linear Coefficient ( $\beta$ )Quadratic Coefficient ( $\gamma$ )	2600 (kg/m <sup>3</sup> ) 1473 (K) 7.61 X10 <sup>-5</sup> (K <sup>-1</sup> ) 0.01X10 <sup>-5</sup> (K <sup>-1</sup> ) <sup>2</sup>
3. Thermal Conductivity	Constant (k)	$2 J.m^{-1}.s^{-1}.K^{-1}$
4. Heat Capacity	Constant $(C_p)$	1200 $J.kg^{-1}.K^{-1}$

Table 6.1: The physical properties for modelling Colombia River Basalts (CRB) magmas

Table 6.2: The Physical properties used for the country rock model

Continental Crust physical properties	Values	
Density	2850 ( $kg.m^{-3}$ )	
Thermal Conductivity	2.5 $(J.m^{-1}.s^{-1}.K^{-1})$	
Heat Capacity	1170 $(J.kg^{-1}K^{-1})$	

#### 6.2 The Boundary and initial conditions

It is important to mesh the model first before applying boundary and initial loads to obtain a solution. Both the magma chambers and country rock were meshed. Zero velocity wall boundary conditions (includes no-slip boundary conditions) were applied to the exterior nodes of all the magma chambers (for example, see figure 6.1). Further, this stipulates that no fluid leaves or enters the magma chamber. The initial condition

temperatures used for all the magma, that is, for the intrusive melts and the magma chambers without the country rock, were applied to all nodes in the beginning of the first time step and allowed to change upon cooling.



The country rock used in this thesis is extended from the surface of earth to a depth of 3km down from the surface. The upper and bottom surface boundary temperatures used for the country rock simulated a geothermal gradient with temperatures rising with an increase in depth at a rate of  $30^{\circ}$  C.km<sup>-1</sup>. Zero heat flux was assumed along the side-walls of the country-rock to simulate adiabatic walls with no heat leaving the country rock system (see figure 6.1 and table 6.3 for details on the initial and boundary conditions used). Only 2-D calculations were performed. Along the surface of the country rock an ambient temperature ( $20^{\circ}$ C, i.e.  $\sim$ 300K) at normal atmospheric pressure of 101.325KPa was applied to simulate atmospheric conditions. These surface boundary temperatures are

temperatures are similar to those used by Hayba and Ingebritsen (1997) since they were applied to simulate heat conducted into the country rock from the deeper parts of the warmer crust. The top surfaces of all the magma models are emplaced downwards to a depth of 1km below the surface of the earth. The depth thickness for the magma models from their roof varies with 1.76 km for model 1, 1.69 km for model 2, 1.63 km for model 3 and finally a depth 1.69km for model 4.

Boundary and Initial Conditions	Magma Chamber	Country Rock
Boundary Conditions	Velocity: $V_x = 0, V_y = 0$ Fixed temperature: 800 °C (1073 K)	Temperature: Top surface = $20 \ ^{\circ}C$ (~ 300K) and a Geothermal Gradient of $30 \ ^{\circ}C.km^{-1}$
Initial Conditions	Temperature:         1200 °C           (1473 K)         1200 °C	Temperature: Geothermal Gradient of 30 °C. km <sup>-1</sup>

Table 6.3: The initial and Boundary conditions for 2-D magma and country rock models

The reasons for such extensions are outlined in chapter 1.1 of this thesis. The magma models used were completely surrounded by the country rock. This was done to gain a better insight of the magma processes during crystallization. The next section contains figures of all the magma and country models used in the analysis that is, mesh sizes, mesh types and element types.

# 6.3 The Models

#### 6.3.1 Mesh control

Most of the finite element analysis models are built using a solid model or geometric model. The Computer Aided Design (CAD)-type representation of the structure defines the geometry to be filled with nodes and elements, which are used to facilitate applying loads or other analysis data. It is only possible to obtain a solution when all the analysis information is transferred to the finite element analysis (FEA) model. Meshing is

therefore defined as a process of creating a finite element model (nodes and elements) from a solid model (see the introduction to Ansys 5.3, 1996). The Ansys mesh controls are the most important step in the analysis because the decisions made at this stage in model development will profoundly affect the accuracy and the economy of the analysis. It allows one to establish factors such as the element shape, mid-side node placement and the element size to be used in meshing the solid model (see documentation on Ansys 5.6, 2000).

#### 6.3.1.1 Ansys Mesh Tool

The Ansys mesh tool provides a convenient path for common mesh controls, as well as most frequently performed operations. The mesh tool is an interactive 'tool box'. There are many different functions available on the mesh tool to control size; a few of these are listed below. The reader is urged to see Ansys 5.6 (2000) online document for details.

- · Controlling 'Smart --sizing' levels
- Setting element size controls
- Specifying meshing type (free or mapped)
- Refining meshes
- "Global" element sizing

There are several reasons why differing or mixed mesh sizes have to be chosen to control an analysis (see, Ansys 5.6 (2000) online documentation and the introduction to Ansys 5.3, 1996). The 'smart-sizing' element is the newest and most effective of these controls. The smart element sizing meshing feature creates initial element sizes for free meshing operations providing a range of setting from coarse to fine mesh. The setting range is between 1 for extremely fine mesh and 10 for a very coarse mesh. However, it is recommended to stay within the range of 4 to 8 (Ansys 5.3, 1996; Ansys 5.6, 2000). To illustrate this operation for instance, if smart sizing is used on a model that contains only an area, Ansys will use the area to calculate the guiding element size that it should use to mesh the model. Alternatively, if 'smart-sizing' is used on a model that contains both an area and a volume, Ansys uses the volume to calculate the guiding element size for the model, even if the area in the first model (area only) and the area in the second model (area and volume) are exactly the same and the 'smart sizing' setting is the same. Therefore, the elements Ansys uses to mesh the first model (area only) will not be as coarse as the elements it uses to mesh the second model (area and volume) because Ansys attempts to prevent volumes being meshed with too many elements (Ansys 5.6, 2000). The global element size operation was used in this thesis to prevent the latter problem, because the use of global element size ensures that the size of the elements remains the same for both the country rock and magma models. In this study 40-mesh element size for all the models were used for both the magma chambers and the country rock. The mesh element sizes used for this thesis were based on the calculations done by Harrison (1998). The mesh refinement experiments performed by the latter author tested the effects of mesh refinement on solution accuracy (see Harrison 1998, for details).

In finite element calculations the solution accuracy is based on mesh sizes; the finer the mesh, the higher the solution accuracy.

#### 6.3.1.2 Free or Mapped Meshing

Ansys emphasizes the importance of choosing the type of meshing (free or mapped) to be used for a model. 'Smart-sizing' can be activated for both free and mapped meshing for quadrilaterals and triangles. However, the "Smart-sizing' should be deactivated when meshing hexahedral and tetrahedral elements. Ansys can only map mesh hexahedral elements and only free mesh tetrahedral elements, it cannot perform the reverse to both elements. The magma models used for this research had irregular or complex geometries. Ansys could not perform a global element size control on the models using the quadrilateral element type of shape to produce a mapped mesh so it was required to perform a free mesh in these models.

#### 6.3.1.3 Mesh Refinement

In a local region, a mesh refinement can in general be done in either of these two situations listed below:

• In specific regions of the model where you would like to have a finer mesh, or

• After you have completed the results of the analysis and would like more detailed solution in the regions of interest

Ansys allows mesh refinement for all areas; volume meshes composed of tetrahedra and also around local specified nodes, elements, keypoints and lines. However, Ansys does not allow local mesh refinement for volume elements other than tetrahedra. The level of the mesh refinement can be specified from 1 to 5. The value of 1 provides a minimal and a value of 5 a maximum refinement. These refinement values have different element edges for the refined region. For example, level 1 has an element edge of approximately half the original edge lengths and level 9 has an element edge length of one-ninth the original edge lengths (see Ansys 5.6, 2000, for details). An element mesh refinement of level 2 and edge element of one third was applied to magma model 1 for the present calculations. See figure 6.2. Figure 6.2 is the model of the magma chamber with a free mesh of a global element size with 40 edge elements prior to the mesh refinement operation. Whereas in figure 6.3, the magma chamber is meshed refined with line elements along the walls, sides, top and bottom surface. The importance of the mesh refining operation cannot be over emphasized. Ansys clearly states that during the mesh refinement operation it is standard practice to put more elements in a region with higher solution gradients. Sufficient mesh densities are required to enable the program to capture the finer details of the nature of the phenomena investigated. The higher the mesh density over those regions; the better the results. There is a distinct difference with meshes in both models of figure 6.2 and 6.3, since in figure 6.3 one can clearly observe the impact of the mesh refinement operation. The mesh refinement was only performed on the first model of the magma chamber in figure 6.3. This was only for illustration purposes. However, mesh refinement has the disadvantage of consuming computational time, hardware resources and computer memory, hence the mesh size of 40 global edge element size used for rest of the calculations.

This choice arises from the mesh refinement experiments done by Harrison (1998), which provide a good rationale for not using the mesh refining operations in the present calculations.

CANSYS Graphics E





Figure 6.2: A free quadrilateral element mesh of Magma Chamber model 1. This model contains no mesh refinement. The model has been meshed using the latest Ansys5.6 version

Figure 6.3: Mesh refined magma model 1. The line element mesh refined operation was performed along the walls, the sides and the top surface of the magma.

#### 6.3.1.4 Interior mesh: Mesh expansion control and transition

The mesh expansion option of Ansys can be used to control an interior area of the model if there are no lines to guide the size of the mesh. This command is used to guide the mesh from a fine mesh on the boundary of an area to a coarse mesh in the interior. The transition option operation is used to control the rate of transition from fine to coarse element. The expansion option is used to size the internal element in an area based on the size of the element on the area boundaries. The value, which is the expansion or contraction factor, ranges from 1 to 4. If the value is less than 1, a mesh with smaller



Figure 6.4: Magma model 2 with a quadrilateral free mesh. The right left limbs and bottom thickness is 450m. The depth from the top surface to the bottom is 1.69km

elements in the interior will allowed. Values for this option, should be greater than 0.5 but less than 4. However, the mesh transition option controls how rapidly the elements are allowed to change in size from the boundary to the interior. For the best results, the value must be greater than 1 and be less than 4 (Ansys 5.6, 2000). The mesh size, mesh refinement and mesh distribution was controlled rigorously in this study.

#### 6.4 Model Structure

Only the first magma model without surrounding country rock was mesh refined. The calculations were performed as an illustration to show the impact of mesh refinement on physical processes such as the convection of fluid, wall shear, temperature distribution and fluid velocity of the magma chamber upon cooling. However, most of the calculations performed on the other rest of the models with and without the country rock were without mesh refinement. The figures 6.4 to figure 6.6 are meshed models of magma chambers used with different geometries. The magma chamber models are emplaced 1km deep from the top surface of the earth crust. The top surfaces of the magma models are 2.6 km in length extending from the center of the country rock to the sides. The figures 6.7 to 6.10 show two-dimensional rectangular meshed models of



Figure 6.5: Magma model 3. With thickness of 650m along the right and left limbs and the bottom surface. The depth thickness from the top of the surface to the bottom is 1.63 km

Figure 6.6: Magma model 4. The thickness along the left and right side walls and bottom surface now extended to 950m. With a depth thickness of 1.54 km from the top surface to the bottom.

country rock with a breadth of 6 km for the top and bottom surfaces and a depth of 3 km down from the surface of the earth crust, with a total area of  $18 \text{km}^2$ . The magma models had 40 elements along each edge and consequently the inner edges of the country rock also had 40 elements each. The procedure was that contact surface nodes on the magma chamber and the country rock coincide. The magma chamber models in figures 6.2 to 6.6 fit exactly into the central cavities of country rock models in figures 6.7 to 6.10.

For simplicity, linear equations were employed in the exposition of the finite element methods chapter 5. The equations of fluid mechanics are non-linear and their treatment by finite elements can be found in many texts such as Wang and Anderson (1982). The results obtained in sections 7.2 and 7.3 include variable viscosity and density. The latter results were obtained by employing the Ansys Sutherland liquid law to calculate the variations in viscosity with temperature or vise-versa. The second order polynomial was employed to compute the density variations with temperature. The thermal conductivity was assumed constant (Ansys 5.7 online document 2000). The non-Newtonian Power Law viscosity model was used to obtain the results shown in sections 7.4 and 7.5 because the Sutherland liquid law is restricted to Newtonian fluids. Hence, by using Ansys 5.6 Sutherland liquid law could not be utilized to calculate the shear distribution within the magma. The UserVisLaw (User programmable subroutine) facilitated the usage of the Power law to calculate the shear distribution within the magma chamber (Ansys 5.7 online document 2000).



**Figure 6.7**: Country rock model 1. An intrusive system, the void region showing the emplacement of magma model 1 in figure 6.2



Figure 6.8: Country rock model 2 with the empty region indicates the emplacement of magma model 2 in figure 6.4.



Figure 6.9: Country rock model 3 with the empty region emplaced with magma model 3 in figure 6.5.

Figure 6.10: Country rock model 4, the empty region emplaced with magma model 4, in figure 6.6

## Chapter 7 Results

#### 7.1 Geothermal Gradients

The earth's surface wall boundary temperature used was  $20^{\circ}$ C (~300K) simulating ambient air or standard atmospheric conditions. A geothermal gradient of  $30^{\circ}$ C/km from the surface to 3km downwards to the bottom of the country rock was applied. The geothermal gradients simulate the temperature distribution within the country rock before magma emplacement. Steady-state computations were performed using the Ansys 5.6 Flotran code to generate the geothermal gradients. The geothermal gradients of the models M1 to M2 are displayed in figures 7.1, .7.2, 7.3 and 7.4 below.



Figure 7.1: Geothermal Gradient; model 1(M1)



Figure 7.3: Geothermal Gradient; model 3(M3).





Figure 7.4: Geothermal Gradient; model 4(M4).

### 7.2: Velocity and temperature distribution profiles for model 2 (M2)



Figure 7.5: Velocity profile, 1 year.

Figure 7.6: Velocity profile, 10 years



Figure 7.7: Velocity profile, 20 years.



Figure 7.8: Velocity profile, 30 years.



Figure 7.9: Velocity profile, 40 years.



Figure 7.10: Velocity profile, 50 years.



Figure 7.11: Velocity profile, 60years.





Figure 7.13: Temperature profile, 1 year.

Figure 7.14: Temperature profile, 10 years.

- 0



Figure 7.15: Temperature profile, 20 years.





Figure 7.17: Temperature profile, 40 years.



Figure 7.18: Temperature profile, 50 years.



Figure 7.19: Temperature profile, 60 years.



Figure 7.20: Temperature profile, 62 years.



Figure 7.21: Temperature profile, 100 years.



Figure 7.22: Temperature profile, 560 years



Figure 7.23: Temperature profile, 1060 years.

Figure 7.24: Temperature profile, 2557 years.



Figure 7.25: Temperature profiles, 5063



Figure 7.26: Temperature profile, 9018 years.

7.3 Temperature and velocity distribution profiles for model 4 (M4)





7.27: Temperature distribution in 1 year



Figure 7.29: Temperature profile in 10 years

7.28: Velocity distribution profile in 1 year



Figure 7.30: Velocity profile in 10 years



Figure 7.31: Temperature profile in 20 years



Figure 7.33: Temperature profile in 30 years



Figure 7.32: Velocity profile in 20 years



Figure 7.34: Velocity profile in 30 years



Figure 7.35: Temperature profile in 40 years



Figure 7.37: Temperature profile, 50 years.



Figure 7.36: Velocity profile in 40 years



Figure 7.38: Velocity profile, 50 years.


Figure 7.39: Temperature profile, 60years.



Figure 7.40: Velocity profile, 60 years.



Figure 7.41: Temperature profile, 64 years.



Figure 7.42: Velocity profile in 64 years



Figure 7.43: Temperature profile, 100 years.



Figure 7.45: Temperature profile, 1060 years.



Figure 7.44: Temperature profile, 560 years.



Figure 7.46: Temperature profile, 2560 years.



Figure 7.47: Temperature profile, 5060 years

Figure 7.48: Temperature profile, 10000 years.



Figure 7.49: Temperature profile, 15000 years.

Figure 7.50: Temperature profile, 20000 years.



Figure 7.51: Temperature profile, 25000years.



Figure.7.52: Temperature profile, 30000 years.



Figure 7.53: Temperature profile, 40000 years.



Figure 7.54: Temperature profile, 50000 years.

# 7.4 Shear distribution for a fixed geometry: Model 2 (M2)

Note: the meaning of the circled numbers 1,2,3,4,5,6,7 and 8 are explained in the discussions and conclusions text of sections 8.2 to 8.3.1.



Figure 7.55: Velocity distribution profile for 1 year.



Figure 7.56: Shear distribution profile for 1 year.



Figure 7.57: Velocity distribution profile for 10 year.



Figure 7.58: Shear distribution profile for 10 years.



Figure 7.59: Velocity distribution profile for 20 years.



Figure 7.60: Shear distribution profile for 20 years.



Figure 7.61: Velocity distribution profile for 50 years.



Figure 7. 62: Shear distribution profile for 50 years.



# 7.5 Velocity and shear distribution profiles for variable geometry





Figure 7.64: Shear distribution profile for 50 years; Model 1 (M1).



Figure 7.65: Velocity profile for 50 years; Model 2 (M2).



Figure 7.66: Shear distribution profile for 50 years; Model 2 (M2).



Figure 7.67: Velocity distribution profile for 50 years; Model 3 (M3)



Figure 7.68: Shear distribution profile for 50 years; model 3 (M3).



Figure 7.69: Velocity distribution profile, 50 years: Model 4(M4)



Figure 7.70: Shear distribution profile for 50 years; Model 4 (M4)

# **CHAPTER 8**

# DISCUSSIONS AND CONCLUSIONS

## 8.1 Discussion 1: Velocity and Temperature distribution for Models 2 and 4

The velocity distribution simulation results for these very small magma chambers indicate that they stop convecting at an early period during cooling. The total period taken by the magma in model 2 to transfer heat and mass through convection is approximately 62 years, after this time no further convection is observed. The heat was transferred to the surrounding country rock by conduction only. The same behaviour was observed for model 4 with an extended geometry at the side limbs and bottom. The size for the latter model is almost doubles that of model 2. The results showed convection for model 4 lasted only for about 64 years. This is intriguing because, for such a larger geometry, convection is intense initially, but it takes almost the same time as model 2 to cease. However, the results are feasible because the heat transfer is dependent on the Rayleigh number. The depth  $(d^3)$  is the determining parameter because of its third order influence in the Rayleigh number (see section 4.2.1.1, equation 4.57) and the larger size implies higher heat transfer. However, the magma viscosity overrides the effect of size. Ansys 5.6 computed the variable viscosity of magma from an exponential temperature dependent relationship that includes the effect of suspended crystal content (see equation 3.15 section 3.3.1.3). The viscosity 'gums' up the magma during the first years of the cooling, hence overriding the effect of the inertial terms in the Navier-Stokes equations. However, upon cooling, the time taken for heat transfer by conduction is approximately six times for magma model 4 than for model 2. The present results reveal the cooling time for Model 2 is about nine thousand years and fifty thousand years for model 4. The results shows that the ratio of the calculated cooling times for model 4 to model 2 are approximately the same as the e-folding times. The vector velocity profiles for the fluid flow in magma model 2 from the first year to 62 years are displayed in figures, 7.5, 7.6, 7.7, 7.8, 7.9, 7.10, 7.11 and 7. 12. For the first year, the upper left and right limb contain blue regions indicating zero velocities. The fluid cools fast in the upper limbs. The central zones cool slower and have a high velocity, hence the stronger convection. Figure 7.5 and 7.6 displays a turbulent velocity vector profile for the first 10 years, with a maximum velocity with magnitude of about 0. 00142 m/s. However, for the next 20 to 62 years, figures 7.7 to 7.12 display a weaker turbulence the flow that gradually becomes more laminar. The maximum velocity has decreased to a low value of 0.00064 m/s at the center, with zero velocity vectors almost in the entire magma domain. For magma model 4 (M4), figures 7.28, 7.30, 7.32, 7.34, 7.36, 7.38, 7.40, 7.42 indicate the vector velocity profiles in the magma chamber, for the duration of one year to 64 years. Initially, that is from the first to the tenth year, maximum vector velocities of value 0.0019 m/s are displayed in figures 7.28 and 7.30, indicating regions of the strongest convection. The velocity magnitude is higher than those found in model 2 (M2) for the same time. However, for the next 20 to 30 years (figures 7.32 and 7.34) high velocities are still observed in model 4 still indicating stronger central convection. For the next 40 to 64 years the decreasing values in velocity (figures 7.36 to 7.42) show convection is dying out with the maximum velocity dropping to 0.00064 m/s in 64 years after which the fluid no longer convects. Intriguing convecting behaviour is observed in model 4. During cooling the fluid velocity plots reveal convection cells that sways from left to right in the upper limbs of the magma. However, at 62 years the convection resumes the same symmetry observed in the first year. Model 2 maintains the initial symmetry throughout the 62-year period of convection. However, all the calculations show the magma velocities for both models to display a similar fluid flow pattern. The temperature distribution profiles for model 2 are displayed in figures 7.13, 7.14, 7.15, 7.16, 7.17, 7.18, 7.19, 7.20, 7.21, 7.22, 7.23, 7.24, 7.25 and 7.26. Those for model 4 (M4) are displayed in figures 7.27, 7.29, 7.31, 7.33, 7.35, 7.37, 7.39, 7.41, 7.43, 7.44, 7.45, 7.46, 7.47, 7.48, 7.49, and 7.50. These results were all calculated from the first year to the time required for the magma to reach the maximum e-folding cooling temperature. The maximum efolding cooling temperatures is calculated using the following relationship (Kreith and Bohn, 1993)

$$T_{\text{max:cooling}} = \frac{1}{e} \left( T_{\text{initial}} - T_{\text{wall}} \right) + T_{\text{wall}}$$
(8.1)

The value calculated for all the models is about 763 K.

#### 8.1.1 Conclusion 1

During the initial stage of cooling, convection is vigorous for both magma models but it is much stronger for magma model 4 than model 2. The time taken for both magma models to stop convecting is approximately the same. This work concludes that the time taken for both of the magma chambers to convect is not dependent on the size  $(d^3)$ because the viscosity overrides the effect of size. However, magma models of bigger geometries take a longer time to lose heat through conduction than those with small geometry. For instance, magma model 4 took about six times longer than model 2 to cool to the e-folding temperatures.

### 8.2: Discussion 2: Shear and velocity distribution for fixed geometry

Velocity and shear distributions for model 2 (M2) are shown in section 7.4 7 of chapter 7 by figures 7.55 to 7.62. These velocity and shear distribution profiles were calculated from the first year to 50 years at the different time steps. The first ten years are chaotic. The high velocity (arrow 3) and high shear (arrow 6) profiles in figures 7.55 and 7.56; simulate a random distribution within the center of the magma chamber during the first year. After ten years the high velocities and shears (shown by arrows 6 and 4 in the previous figures, i.e. 7.55 and 7.56) migrate to the bottom limb sidewalls (see arrows 3 and 8 in figures 7.55 and 7.56). The distribution of low velocities and shears are shown by (arrows 2 and 5) in figures 7.55 and 7.56, respectively. For the first year, convection is intense because of the high temperatures at the initial stages. After 10 years, the arrows 2 and 3 in figure 7.57 show high velocities distribution profiles at the upper and the bottom sidewalls, whilst the high shear zones in figures 7.58 are indicated by (arrows 5 and 8 respectively). During this time the turbulence sinks down the upper to the bottom sidewalls. The approximate zero velocity profiles (arrow 8) in figures 7.55 and 7.57 correspond to zero shear zones (see, arrow 6, all the dark blue regions) and the light blue, or pink regions (arrow 7) are low shear distribution zones. The light blue/pink regions indicated by (arrow 7) are results of hot lighter magma rising from the floor of the bottom limb through the center to the rooftop of the upper limb where it cools (dark blue colours), becomes heavier, sinks down the sidewalls.

The next 20 to 50 years, velocity profiles are higher at the bottom limb walls (arrow 3) than those in the upper limb walls (arrow 2) in figures 7.59 to 7.61. Here, the high velocity profiles (arrow 3) decrease respectively with an increase in time, and so does the high shear zones (arrow 8) when compared to the shear zones at the walls in the upper limbs (arrow 5) [see figures 7.60 to 7.62]. Consequently, the increase in time also results to a steady disappearance of low shear zones (arrow 7) in the center of the magma during cooling.

# 8.2.1 Conclusion 2:

1) During the first year the fluid motion is highly turbulent and chaotic, high velocities and shears are only prominent in the center and no high velocities and shear are seen at the walls of the magma chamber.

2) The large dark blue regions (arrow 1) represents approximately zero velocities, hence the zero shears (arrow 4). Simultaneously, the sidewall velocities decrease resulting in low wall shear. The decreases in wall shear result in the concentrate building up and an increase in size of particulate matter toward the center of the upper limb. The center of upper limbs contains sulphide melts with dilute concentrate of the PGEs because the free PGEs have already precipitated.

3) The free PGEs are the first to freeze out because of their high melting temperatures. The zones of zeros shear as shown by arrows 6 in figures 7.58, 7.60 and 7.62 would theoretically host the PGEs during the first 10 years. The high shear observed at the roots of the dykes/sills scavenges the free PGEs to the zero shear zones. The dispersive pressure (Bagnold effect) drives particulate aggregation from both sides of the walls into zones designated by arrow 6. During the next 50 years the PGEs concentrate, the increasing viscosity of the magma 'locking' them into place.

#### 8.3 Discussion 3: Velocity and shear distribution profiles for variable geometry

The figures 7.63 to 7.70 in section 7.5 of chapter 7 show the velocity and corresponding shear distribution profiles of magma flow in variable geometry. The arrows in figures 7.63, 7.65, 7.67 and 7.69 indicate different regions of the convecting velocities of the magma. Arrow 3 indicates the regions of high velocity. Arrow 1 indicates zero or negligible velocities hence, little fluid motion. Finally, the low velocities are shown by (arrow 2). However, for the shear distributions it is important to note that the small sized geometry of figure 7.64 led to the absence of high shear zones on both walls of the bottom limbs, therefore, no zero shear zones are eminent /seen in the middle of the walls hence, arrow 6 is not shown. Arrow 8 in figures 7.64 to 7.70 indicates the transition in regions of high shear distribution on the walls, that is, from one wall (see figure 7.64) to both walls (Figures 7.66, 7.68 and 7.70). A respective decrease in the high shear profile is shown by (arrow 8) from figure 7.64 to 7.70. However, the opposite behaviour is seen for the high shear distribution shown by arrow 5. Here, the shear distribution increases from 7.64 to 7.70, respectively. This is because of the increase in geometry size of the magma chamber, which results in stronger convection, hence the higher shear. The regions shown by arrow 4 (dark blue coloured) are zones of zero shears. The zones of zero shears shown in figures 7.64 to 7.70 become more pronounced in the upper limb of the magma chamber when the geometry is varied. This is because of the cooled upper regions of the magma, hence zero fluid velocity. The regions shown by arrow 7 are low shear zones. They result from hot magmatic fluid flowing from the bottom, upward cool and then sink down at the sidewalls. The strongest circulation is through the center to the rooftop. This results in mild shear migration (arrow 7) into the upper limb from the floor of the magma chamber.

All these calculations are carried to 50 years cooling history only. The free PGEs freeze out of the melt during the first 10 years because of their high melting temperatures (see the zero shear regions shown by arrow 6 in figures, 7.66, 7.68 and 7.70). After approximately 50 years of cooling, many of the PGE's would have scavenged into sulphides and/or, concentrated and 'glued' in the zero shear zones as shown by arrow 6

because of the increasing viscosity. The dispersive pressure of magma, and the flow pushes the PGE's to the zero shear location from both sides of high shear zones.

# 8.3.1 Conclusion 3

After about the first 50 years; the PGEs are locked into zero shear zones shown by arrow 4 in figures 7.66, 7.68 and 7.70 due to increasing viscosity that 'glues' them into place. The low or zero shear zone shown by arrow 6 at the bottom is much smaller, the PGEs are therefore less dilute, hence more likely economical. The effect of increasing the magma chamber size enhances convection, hence increasing the collision rates between the immiscible sulphides and the PGEs resulting in increased shear aggregation, hastening particulate matter concentration during cooling. The increased sizes leads to maximum scavenging and large low to zero shear zones in the upper limbs of the magma chamber. PGEs hosted in these large zero shear zones are the most dilute PGEs, hence least economical.

### 8. 4: Animations

The animations provided with the thesis are on CD; they simulate the time evolution during cooling process of the magma chambers, surrounded by the country rock. Two models with both variable viscosity and density (see equations 3.15; 3.17 and the graphic display of the data in figures 3.4 and 3.5 respectively) were used to demonstrate the impact of varying the geometry of the magma chambers on the time evolution of heat mass transfer of magma. The animations results are the velocity and temperature distribution profiles are shown in sections 7.2 and 7.3. The animations are:

#### 1.Model 2 (M2):

- (i) Temperature contour animation in a T-shaped magma chamber and the surrounding rock (Filename: Rock 2. avi).
- (ii) Velocity vector animation in T- shaped magma chamber and the surrounding country rock (Filename: Vel 2. avi).

# 2. Model 4 (M4):

 (iii) Temperature contour animations in T – shaped magma chamber and the surrounding country rock (Filename: Rock 4.avi)

These temperature animations results; reveals small and steady drop in the magma temperature for the first 100 years. Followed by large drops in magma temperature contours on further cooling. This is because, initially, the drop in magma temperature was calculated at successive and constant one-year time interval steps for 100 years. The purpose was to capture the velocity profiles before convection stops. Thereafter, the magma was allowed to cool for large and unsteady time intervals that is 560, 1060 years etc., (see, the results in section 7.3).

 (iv) Velocity vector animation in a T-shaped magma chamber and the surrounding country rock (Filename: Vel 4. avi).

### 8. 5: Future Research Initiatives.

The magma model geometries used for these calculations, although simplified, represents a step-by-step approach towards more realistic models of complex intrusions such as the Great Dyke of Zimbabwe. These results are helpful in laying a good foundation for broader and more realistic inferences could be drawn. This effort would aid in throwing light on estimating reserves and locating minerals of economic importance. The following further the research is indicated.

1. Finite Element computations to determine the areas of zero shear, hence the location of economic minerals for realistic 3-D magma models of the Great Dyke of Zimbabwe with the inclusion of variable temperature dependent viscosity.

2. Application of discrete element methods for granular flow, to visualize the shear aggregation on high shear zones, concentrates and 'gumming up' of PGEs particulate matter in zero shear zones. In discrete element method the full physics of the collision of

many particle will be modelled. It models the interacting forces at local level and deals with rolling and sliding in a way that cannot be described by continuum methods.

3. Location of mineral deposit by chemical transport in the mafic and ultramafic sequence by hydrothermal circulation through porous country rock media by employing finite element calculations for realistic model of the Great Dyke of Zimbabwe.

4. Performing, realistic computational simulations for the cyclic layering of the sequence rocks in the Great Dyke of Zimbabwe, as such will develop more insight into the location and distribution of minerals of economic importance, since most of the minerals are in these cyclic layers.

5. All future work will include phase change, variable specific heats, non-Newton behaviour to account for the yield strength and the formation of crystal load content below the liquidus. Most magmas are non-Newtonian.

Computational fluid dynamics is a fast developing field worldwide, hence a research effort of this nature is highly recommended. It is fast, efficient, cost effective and rewarding. It has a variety of industrial applications for a range of engineering, chemical and multi-physics disciplines. For example, some of the disciplines where CFD is applied are; Electrodynamics, Computational Exploration Geodynamics, Aerodynamics and Structural mechanics. The research builds on the computer technical skills required to develop the human resource of South Africa. South Africa is rich in mineral resources, but because of the lack of technology, much of these resources are still unexplored, hence the future of South Africa lies in manpower with such technical skills

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# **Glossary of Terms**

Alkali basalt: A fine-grained, dark coloured, volcanic rock characterized by phenocryst of olivine titanium-rich augite, plagioclase and iron oxides. For similar  $SiO_2$  concentrations, alkali basalts have a higher content of  $Na_2O$  and  $K_2O$  than other basalt types such as tholeiites.

Archean: One of the three subdivisions of the Precambrian, lasting from about 4000 to about 2500 Ma.

**Basalts:** Refers to a dark coloured, fine-grained, extrusive igneous rock composed of plagioclase feldspar, pyroxene and magnetite, with or without olivine. Most basalts contain phenocryst of olivine, plagioclase feldspar and pyroxene. Basalts are divided into two main types alkali basalts and tholeiites.

**Biotite:** a widespread rock-forming mineral,  $K(Mg, Fe)_3 AlSi_3O_{10}(O, H, F)$ .

**Boundary layer:** is defined as the region near the wall where the convective velocities decrease to zero from mainstream.

**Bronzite:** An orthopyroxene with the formula (Mg, Fe)  $SiO_3$ , with about 70-90% of magnesium content and also belongs to the pyroxene group of silicate minerals. It is found in basic and ultra basic igneous and metamorphic rocks.

**Chromite:** The primary source of chromium, which occurs in basic and ultra basic rocks, it's a member of spinel group of minerals, FeCr<sub>2</sub>O<sub>4</sub>

**Convective Scavenging:** The mechanism for concentrating suspended crystal loads (phenocrysts) in zero shear zones.

Country rock: The environs surrounding a magma chamber (see magma chamber).

Crust: approximately the uppermost 30 kilometers of the Earth.

**Cumulate:** Applied to igneous intrusive rocks formed by the accumulation of crystals as a result of gravity settling. The early-formed minerals are called cumulus minerals and show a regular variation in composition with their height of intrusion. It is typical of layered intrusions and common in some differentiated meteorites.

Dunite: Coarse grained, igneous rock, consisting mainly of olivine.

**Dyke (Dike):** Refers to a cross cutting or tabular intrusion. Most dykes are vertical or near vertical intrusion through the overlying country rock.

**Eutectic point:** Refers to the temperature at which this simultaneous crystallization occurs.

**Eutectic systems:** a mixture of two or more minerals in definite proportions with each mineral crystallizing simultaneously from the melt.

**Gabbro:** A coarse grained, basic igneous rock, consisting of essential calcium-rich plagioclase feldspar (approximately 60 %), clinopyroxene (augite or titanaugite), and orthopyroxene (hypersthene or bronzite) plus or minus olivine with accessory magnetite or ilmenite. The gabbros result from the slow crystallization of magmas of basaltic composition and can be divided into the tholeiitic and alkali types.

Greenstone belt: Refers to a large geologic formation up to 250km across, which is largely of Archean age.

Hypabyssal: A medium- grained, intrusive igneous rocks, which have crystallized at shallow depth (no defined/agreed depth limit to the term shallow) below the Earth's surface.

Igneous: Refers to rocks that have crystallized (solidified) from magma.

Intrusive, intrusion: is a body of rock, usually igneous that is emplaced within preexisting rocks.

Layering: Refers to different layers of igneous intrusion, which are different in mineralogical compositions, sometimes called rhythmic layering.

Liquidus: is the temperature range at which crystallization starts to occur.

Lithology: The description of the macroscopic features of a rock, e.g. its texture or petrology.

Mafic: Any igneous rock that has a high proportion of pyroxene and olivine.

**Magma:** A hot, silicate, carbonate, or sulphide melt containing dissolved volatiles and suspended crystals, which are generated by partial melting of the Earth's crust or mantle and is the raw material for all igneous processes.

Magma Chamber: A region postulated to exist below the Earth's surface, which hosts' magma injected from the deeper crust or upper mantle. The magma is either, stored, or moves to the Earth's surface at the side of the volcano.

Magmatic differentiation (magmatic fractionation): Formation of a variety of rock types from an initial single parental magma.

Mantle: That portion of the Earth lying between its crust and its core, approximately 2300 kilometers thick.

Mineral deposit: Refers to any natural and a local restricted concentration of minerals in the Earth's crust.

Ore deposit: It is a mineral deposit in which the mineral concentration contains substance that is of economic interest to concentrations that rich enough to warrant mining.

**Orthopyroxene:** Refers to a series of pyroxenes, which crystallize in the orthorhombic system. They consist of enstatite (MgSiO<sub>3</sub>) and ferrosilite (FeSiO<sub>3</sub>) end members.

**Paleomagnetism:** Refers to the Geophysics of measurement and interpretation of remnant magnetism or the record of the earth's past magnetic field (for example, polar wandering and continental drift).

**Plagioclase feldspar:** Refers to one of the most important rock-forming silicate minerals with the general formula (Na, Ca)(Al)<sub>1-2</sub>(Si)<sub>2-3</sub>O<sub>8</sub>. The solid solution series is between the two end-members *albite* (NaAlSi<sub>3</sub>O<sub>8</sub> and the *anorthite* (CaAl<sub>2</sub>Si<sub>2</sub>O<sub>8</sub>).

Plagioclase series: Refers to an isomorphous series of feldspars ranging in

**Plutonic:** A general term applied to a body of intrusive igneous rock which has us crystallized at great depth.

**Poikilitic:** Terminology applied to the texture produced when several orientated or unorientated crystals are enclosed within larger crystals in an igneous rock. The larger crystals have more widely separated nuclei than the closed crystals and may grow faster, hence enclosing the grains.

**Primary migration:** First stage in the upward migration of hydrocarbons within and then out of the source rock..

**Pyroxenite:** Refers to an ultra basic, igneous rock, which essentially consists of clinopyroxene, orthopyroxene and olivine.

**Reserve base:** It is an identified resource base that meets the required physical and chemical criteria related to current mining and production practices, of grade, quality, thickness a and depth.

Rhyolite: Refers to a fine- grained, extrusive, igneous, with a sugar-like texture, containing quartz, alkali feldspar and one or more ferromagnesian minerals.

Silicic: Results from silica  $(SiO_2)$  or quartz. Igneous rocks with high free quartz  $(SiO_2)$  content are usually referred to as silicic.

Sills: A tabular igneous intrusion having concordant (parallel) surface of contact.

Solidus: is the temperature range at which crystallization ends.

S1, S2, S3: An informal terminology used by (Wilson *et al.*, 1989) to refer to sulphide zones of enhanced sulphide content in the Great Dyke of Zimbabwe.

Tholeiite basalt: An abundant, fine-grained, igneous rock consisting of essential calcium-plagioclase, subcalcic augite, and pigeonite, with interstitial glass or fine quartz-feldspar intergrowths. This type of basalt, oversaturated with silica; it occurs as plateau lavas on the continental crust and as the main extrusive component of the ocean floor.

**Ultrabasic:** Refers to an igneous rock that consists entirely of ferromagnesian minerals and possesses no free quartz, which is less than 45 % silica  $(SiO_2)$  ' Ultramafic is a partial synonym'.

Ultramafic: (See Ultrabasic)

# **APPENDIX** A

**Discontinuous** Series

# **Pseudo ternary systems:**



The fractional crystallization process below demonstrates the production of mafic minerals such as olivine, pyroxene, amphibole and biotite. A must crystallize to a mixture of diopside (clinopyroxene), fosterite (olivine) and anorthite (plagioclase), in the proportions fixed by the bulk composition A, for equilibrium crystallization. However, for fractional crystallization the bulk composition of the system can change, depending upon the proportion of solid phases removed from equilibrium with the liquid. For both equilibrium and fractional crystallization the first mineral to crystallize from liquid A is olivine and the residual liquid is driven away from A along the line A-A' until the fosterite-diopside cotectic curve is intersected. Olivine and pyroxene then crystallize together as the temperature falls until the eutectic E is reached, when plagioclase joins the assemblage. In the case of perfect fractional crystallization (Rayleigh fractionation), where magma and crystals are continuously separated, the residual liquid will ultimately attain composition E. This is also the composition of the last dregs of liquid in the case of the equilibrium crystallization. Thus by fractional crystallization processes one

could clearly generate a continuous spectrum of liquid compositions lying along the lines A-A' and A'-E, each of which could crystallize as an igneous rock. If the bulk composition of the liquid were B, the array of possible differentiated liquid compositions would now be B-B'-E, as the sequence of fractionation phases has changed. Path B may schematically represent the differentiation of the tholeiitic basalt and path A of alkali basalt. Such ternary phase diagrams do not quite predict the quantitatively fractionation trends for actual magma composition, as these are multi- component system in which phase relations of the minerals may differ significantly from those of simple systems. However, they are most useful in understanding the chemical consequences of the fractionation processes. The fractionation trends of the magmas cannot be constrained without taking into consideration the changing composition of fractionation phases Wilson (1989). In closed -system fractionation of magma, much of the crystallization will occur along the margins of the chamber. where the steepest temperature gradients and the largest under cooling occur and the nuclei already exist Campbell (1978), McBirney and Noyes (1979). The crystal, which grows on the margins or in thin viscous boundary, layers change composition and the local density of the magma and the melt is convected away from the point of origin. The convection effects consequently depend strongly on the physical properties of the magma, the fractionation density of the crystallizing phases and the chamber McBirney (1980), Sparks and Huppert (1984) and Spark et al., (1984). The model for a closedsystem evolution for magma has some of the following consequences and implications:

• Compositional and thermal gradients can be set up in magma chambers containing initially homogeneous magma, gradients can be such that double diffusive layers can develop, each layer evolve as a chemically independent system. However, when parts of the chamber erupt, there can also be a production of zoned and contained compositional discontinuities.

• After compositional gradients have been established in the chamber, crystallization will occur along the margins and will lead to cumulate varying in composition with position. In mafic intrusions, these layerings which are parallel to the margins will be out of phase to phase layering which is parallel to gravitational stratification in the fluid; hence crystal layers in mafic intrusions could also be influenced by double-diffusive layering (Huppert and Spark, 1984).

• Sidewall crystallization influences immediately only a small proportions of the total magma body; because of selective removal of the compositional boundary layer, this can result in highly fractionated

magmas accumulating at the top, or bottom, of a chamber without requiring large amounts of crystallization. However, crystal settling requires large fractions of the magma chamber to crystallize in order to form highly differentiated melts, these highly differentiated melts form at the top of a chamber at an early stage of a sidewall crystallization (Sparks *et al*, 1984).

• Phenocryst can form internally in a magma chamber at double- diffusive interfaces, where under cooling and super- saturations are the greatest. They can form during the mixing of magma, by erosion of cumulates, and as residual crystals from the source region (restite), once crystals of diverse origins are suspended in the magma, further growth can occur (Sparks *et al.* 1984).

