Evaluation of crustal fluid flow in Mesoarchean granite-greenstone terranes via numerical methods

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Abstract

The movement of material, fluids and heat in geological terranes are at the heart of the Earth’s geological history. Through a given tectonic regime the facilitated movement of matter and energy may form ore deposits. A recent thermo-mechanical experiment was conducted to determine whether the gravity driven tectonic process (sagduction), described for Mesoarchean for granite-greenstone terranes, provided the conditions for ore deposit formation. The results of this numerical experiment indicate that the sagduction process is associated with significant lateral temperatures gradients (\(\sim 26^\circ\text{C/km}\)) therefore providing the heat engine required to develop hydrothermal convection cells necessary for ore deposit formation. This dissertation was undertaken to ascertain the conditions required for the generation of convective cells via a detailed fluid flow investigation.

Two sets of fluid flow simulations were undertaken by a one-way coupling of data and processes. Data from Ellipsis, a thermo-mechanical numerical code, such as Geology, Temperature and Strain-rate served as inputs to SHEMAT, a numerical code to solve fluid flow related equations. The first set of simulations serviced as benchmark models mimicking a generalised granite-greenstone terrane. Different permeability conditions and geometries were applied to these models with increasing complexity. Rock alteration index (RAI) was applied to characterise the behaviour of convective cells in the context of the changes in thermal gradient. RAI is constrained further to reflect a conservative second order fluid movement (\(10^{-8}\) to \(10^{-10}\) m.s\(^{-1}\)) in a regional and contact metamorphic setting. The second set of simulations was reproduced from the thermo-mechanical experiment of gravity driven
tectonic in a Mesoarchean setting. In this second set of experiment, an evaluation of the dynamic permeability was calculated from strain-rate values generated through the thermo-mechanical simulations. These strain-induced zones act as fluid pathways and improving the model’s ability for fluid convection.

The result of this study show that early time steps of the sagduction process are associated with thermal regimes capable of developing hydrothermal convection cells heavily influenced by permeability conditions. As the deformation process progressed, the greenstone keel is associated with the development of permeability channels that are funneling fluid flow. These strain-induced permeability pathways were associated with an increase of fluid velocity up to three orders of magnitude. As the deformation process proceed the dynamic permeability homogenise in the upper part of the greenstone keel and fluid flow organised into fluid convection cells in the upper part of the model. In the lower part of the model the fluid flow experience unidirectional advective flow. In the final stage of the sagduction process the distribution of the permeability field reduce the development of hydrothermal convection cells possibly following the thermal equilibration over the crustal profile.

Overall, the high geothermal gradient strongly appear to apply a first order control on the fluid flow regime at the various time-steps of the simulation including a combination of advection and convection patterns. However, the results obtained must be interpreted with care and several important limitations will need to be overcome in order to generate fully coupled simulations. The limitations highlighted in this dissertation include amongst others the need for more realistic characterisation of the dynamic permeability controlling the development of hydrothermal system in a crustal setting.
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Chapter 1

Introduction

When geological fortune strikes, rocks formed in the deeper crust can be found at the surface along the modern and ancient mountain belts and orogenic plateaux. Such outcrops are usually achieved through tectonic events, taking up space made either through lateral displacements of the upper crust (boundary forces), downward return flows of the upper crust (body forces), localised erosion, or a combination of both processes. These events enable the movement of material, fluids and heat that have the potential of forming ore deposits. It is therefore critical to understand how crustal fluid and heat transfer processes are activated and to develop a deeper appreciation of the processes associated with the development of ore deposits and mineral systems.

Many economically significant ore deposits are formed by hydrothermal systems, indicating that their genesis is attributed to the transport of solutes and heat by aqueous fluids (e.g. Cox et al. 2001, Sibson 2004, Ingebritsen and Sandford 1999, McCuaig and Hronsky 2014). Advective fluid movement is often referred to as a mechanism essential to ore deposit formation via the concentration of metals and heat. Based on the deposits’ formation depth relative to the local background geothermal gradient (Ingebritsen and Appold 2012), temperatures of the deposits become significantly higher than expected.
Fig. 1.1 Schematic diagram showing the inter-dependence of the components for fluid flow in porous media being inter-dependent to each other. Chapter 2 will address the three components of fluid flow. Chapter 3 will focus on fluid flow and rock permeability through the construction of general models appropriate to the granite-greenstone sagduction setting. Chapter 4 will integrate the time component of a sagduction process. (located outside the box)

The theory that covers the transportation of mass and heat in the geologic systems is known as the theory of fluid flow in porous media. Fluid flow in porous media is intricately complex due to their inter-dependence on the three components: Fluid Flow, Rock Permeability and Heat Transfer (see Fig 1.1). A detailed overview of the theory expounding the current understanding of each component is required (Area 2 in Fig 1.1). Describing the accounts for mass and energy, this overview will introduce the numerical code of choice for subsequent flow experiments.

With the theory of fluid flow in porous media established, the concepts will be applied to the generalised models of increasing complexity in Chapter 3 (Area 3 in Fig 1.1). These changes in permeability geometries are essential in determining the conditions for fluid instability. It starts with a generic isotropic permeability scenario of the Elder (1967) simulation and the application of a pre-defined background permeability by Ingebristen and Manning (1999). Subsequent simulations will mimic fluid flow in granite-greenstone terrane designed as simplified vertical permeability channels. In addition to fluid flow, the rock
alteration index, RAI (Phillips 1991) and a previously published predictive alteration index (Zhao et al. 2000) will be applied to the simulations in order to characterise the mineralisation patterns and hydrodynamic signatures for convection currents.

In Chapter 4 (Area 4 in Fig 1.1), I will apply the insights gathered from the behaviour of convection currents (in Chapter 3) to different time-steps of a complex geologic process through a reproduction of a recent thermo-mechanical experiment of the Mesoarchean granite-greenstone terrane (Thébaud and Rey 2013). Mesoarchean terranes such as the East Pilbara Craton, Western Australia, consists of granite-greenstone terranes (3,720 to 2,830 Myr) unconformably overlain by extrusive magmatic and sedimentary rocks of the Hammersley Basin (2,770 to 2,400 Myr, Fig 1.2) (van Kranendonk et al. 2002). It is one of the few well documented examples of Archean dome-and-basin pattern (Collins et al. 1998, Hickman 1983). Greenstone belts form strongly foliated vertical sheets connected through vertical triple junctions where cigar-shaped constrictional fabrics dominate (Bouhallier et al. 1995, Chardon et al. 1996, McGregor 1951). Although alternative interpretation including metamorphic core complexes formation following crustal thickening (e.g. Zegers et al. 1996, van Haaften and White 2001, Barley and Pickard 1999) and/or the existence of the interference from crustal folding (Blewett 2002) exists, it was proposed that the dome and basin architecture preserved in the East Pilbara Craton resulted from gravitational instability (Thébaud et al. 2013). The East Pilbara Craton is therefore proposed as a significant geological backdrop to study tectono-thermal processes and associated fluid flow in a complex granite-greenstone sagduction setting.

Archean lode gold mineralisations represent a coherent class of gold deposit called "orogenic gold deposit" that developed over a crustal depth range from granulite to sub-greenschist facies environments (crustal continuum model; Groves 1993). Neoarchean lode gold deposits are associated with deep-sourced fluids (i.e. metamorphic, magmatic or mantle derived) channelled along crustal-scale shear zones (Goldfarb et al. 2005, Rey et al. 2003,
Fig. 1.2 (A) Simplified structural sketch of Mount Edgar and Coruuna Down granitic dome complexes and surrounding regions, taken from Thébaud and Rey (2013). Thick dashed lines are characterised by gentle topography and include both granitic rocks (white) and greenstones (grey region). Boxed region (B) indicate location of the Klondike mining district within the Warrawoona Synform (white star) located above the region of the downwelling regions.

The Warrawoona syncline is described as one of the largest mafic-ultramafic-hosted goldfields in the East Pilbara Granite-Greenstone terrane. Gold endowment within the Warrawoona syncline hold evidence for significant fluid-rock interactions within its kilometre-scale shear zone (Fig 1.3). The region has produced 745 kg of Au from 25 kt of ore at an average grade of 29.6 g/t and it has recently increased its Au reserves by 9.95 Mt at 1.0 g/t found at the Klondyke deposit (Huston et al. 2002, Hickman 1983). These gold deposits composed of quartz veins are hosted within the three main shear zones: the Klondyke shear zone, the Copenhagen shear zone and the Fielding’s Find shear zone (Fig 1.3). It has been suggested that the occurrence for these deposits was suggested to be formed via two major hydrothermal circulation events: first, the creation of a high permeability plumbing system from the shear zones and second, a later hydrothermal event for Au enrichment (Thébaud et al. 2008)).

The numerical experiments presented in this dissertation aim at simulating the fluid circulation leading to the mineralisation of the Warrawoona syncline. The output of selected time-steps from the reproduced thermo-mechanical experiment was extracted and translated into a usable format usable by the fluid modelling numerical code. A one-way coupling method was applied to account for the influences of longer geologic processes and the rapid changes in permeability. The novelty behind this approach was to simulate a first order approximation of dynamic permeability with strain-rate as opposed to using constant intrinsic permeability values. Strain-rate was chosen as a proxy to monitor the dynamic competition between crack growth and crack sealing/healing processes (Cox 2002). Although fully
Fig. 1.3 Gold occurrences in the Warrawoona syncline, taken from Thébaud et al. (2008). White regions represent felsic rocks. Pale grey regions represent basalts. Dark coloured regions represent ultramafic rocks. Black dots represent gold occurrences.
thermal-mechanical-fluid coupled solutions do exist (e.g. Hobbs et al. 2000), this will be the first attempt in simulating fluid flow processes in a complex granite-greenstone sagdution.
Chapter 2

Theory on Fluid Flow in Porous Media

2.1 Preamble

The complexity of fluid flow pertaining to mineralisation has been touched by many authors (e.g. Bickle and McKenzie 1987, Bejan 2004, Nield and Bejan 2006, Cox et al. 2005). Fluid flow drivers revolve are relatively well established by hydrogeology. A porous medium is defined as a material consisting of a solid matrix with an interconnected void (Nield and Bejan 2006). The presence of these interconnected voids (or pores) provides the channels for the flow of fluids through the medium. The distribution of these pores with respect to shape and size is highly irregular in natural porous media. These are exemplified within the natural geology such as sandstones, fractured basalts and crystalline granites. These irregularities in pore spaces have a direct influence to flow quantities such as velocity and pressure.

This chapter addresses the theoretical concepts of fluid flow in porous media. It is structured to address the fundamental concept of fluid flow (Darcy’s Law), its limits and its conservation of fluid. In the next section, this chapter addresses the thermal considerations in porous media and the account of energy in a generic model. The chapter ends with the introduction of SHEMAT as the numerical tool to solve the fluid and heat flow based equations, together with the criteria to help achieve numerical stability.
2.2 Fluid Considerations

The fundamental law to describe fluid mobility through any porous medium was conceived by Henry Darcy (1856) with the development of a water treatment system. He determined that fluid flow had been accomplished through differences in fluid pressures at different topographies. Expressed as Darcy’s law \( u \) (m.s\(^{-1}\)) in Eqn 2.1 represents the volumetric flow through a porous medium. \( u \) is evaluated from the ratio of the difference in the fluid pressure gradient and specific weight of fluid, \( \nabla P - \rho g \), and the viscosity of the fluid, \( \mu \) (kg.s\(^{-1}\).m\(^{-1}\)).

As fluids flow through the porous media, the intrinsic permeability of the media, \( k \) (m\(^2\)) greatly determines the magnitude of \( u \). The negative sign in Eqn 2.1 indicates that fluid flows in the direction of opposing regions of pressure. The linear relationship between volumetric flux and hydraulic gradient serves as the fundamental expression to understand fluid and heat transfer in geologic systems.

\[
\vec{u} = -k \left( \nabla P - \rho g \right) \frac{1}{\mu} \tag{2.1}
\]

Darcy’s law was established to be applicable in certain conditions, including: (a) laminar flow in saturated granular media, (b) under steady-state flow conditions, (c) homogeneous fluid conditions, (d) conductive isothermal, (e) incompressible fluids and (f) neglecting kinetic energy (Nield and Bejan 2006). Due to the averaging characteristic based on the representative continuum and the small influence of other factors, the macroscopic law of Darcy remains applicable even to situations that do not correspond to these basic assumptions (Freeze and Cherry 1979): (a) saturated flow and unsaturated flow; (b) steady-state flow and transient flow; (c) flow in granular media and fractured rocks; (d) flow in aquifers and flow in aquitards; (e) flow in homogeneous systems and in heterogeneous systems; and (f) flow in isotropic and anisotropic media.
2.2.1 Limitations to Darcy’s Law

Darcy’s law had been tested over a wide range of conditions with through empirical experiments (e.g. Ward 1964, Bear, Freeze and Cherry 1979). The outcomes of these experiments indicated the law’s shortcomings at sufficiently high volumetric fluxes. At a certain threshold flow rate, the amount of energy lost to turbulence increased significantly. This caused Darcy’s law to over-predict the flow rate associated with the applied hydraulic gradient. Although these instances are deemed uncommon within the subsurface, they can occur near areas of significant permeability (or porosity), such as in carbonate rocks and lava flows.

The dimensionless Reynold’s number, $Re$, is usually used to estimate the applicability of Darcy’s Law. Reynold’s number (Eqn 2.2) is expressed as a ratio of the fluid’s viscosity to the physical parameters of the simulation, where fluid density, $\rho$, volumetric fluid flow per unit area, $u$, the fluid’s dynamic viscosity $\mu$ (kg.m$^{-1}$.s$^{-1}$) and $L$ (m) being the characteristic length of the porous medium. $L$ in granular porous media refers to the mean grain size distribution (although it takes $\sqrt{k}$ [116], where $k$ is the intrinsic permeability of the medium).

$$Re = \frac{\rho u L}{\mu} \quad (2.2)$$

In the upper limits, the transition to non-Darcian flow appears to take place at $Re \approx 5$ (Bear et al. 2012, Freeze and Cherry 1979). This was estimated in the context of fractured media where the permeability is a function of fracture porosity and spacing ($k \sim Nb^3/12$, and where $N$ is the fracture spacing (Snow 1968), $b$ as the fracture aperture and $u$ representing the average linear velocity across the fractures. The $Re$ value in this example was estimated to be 1,000 (Munson et al. 1990). If we evaluate Darcy’s Law with $\rho = 1000$ kg.m$^{-3}$, $\mu = 0.0011$ at 15° C and $L = 0.0001$ m, we will find Darcy’s law starting to over-predict flow rates when $v \geq 0.0055$ m.s$^{-1}$ or $1.7 \times 10^5$ m.yr.

In the lower limits of Darcy’s flow where hydraulic conductivity becomes significantly small, a minimum hydraulic gradient is established. It was suggested that if the characteristic
length is significantly small, fluids start to produce counter-currents along the pore wells to impede fluid flow (Van Dyke 1982). Efforts were made in attempt to characterise these non-newtonian flows as an exponential function (e.g. Swartzendruber 1962), but, this phenomenon is of little importance in the context of mineralising systems as the value will be too small to impact the fluid flow regime (Kuhn and Gnesser 2009).

### 2.2.2 Driving forces of fluid flow

Several drivers of fluid flow exist, each reflective of a tectonic regime. One of the forms is gravity-driven or topographic flow. The preference of fluid flow is determined to flow from regions of higher topography to regions of lower topography (Hubbert 1940). This type of flow is dominant on continental land masses, predominantly at shallow levels, but it also occurs locally at depth (Garven and Freeze 1984[31]). Maximum flow rates of 1-10 m.yr\(^{-1}\) develop within the aquifers, while much smaller seepage rates exist in permeable strate interlayered with aquitards (Graven and Raffensperger 1997). This type of flow is controlled primarily by topography, surface heterogeneity, variable permeability and basin geometry.

The driving force for groundwater flow is expressed as hydraulic head, \(h\) (m), where \(P\) represents fluid pressure, \(\rho g\) is the specific weight of fluid and \(z\) (m) is the topographical height or depth (in simulations). Hydraulic head is quantified in simulations as the depth of the simulation, giving the initial driving force. By recalling Darcy’s Law (Eqn 2.1), the relationship is rewritten to provide two terms; \(\frac{k}{\mu}\) as the volumetric fluid rate through a porous medium and \((\nabla P + \rho g \Delta z)\) to account for the driving force.

Although fluids have a tendency to operate at differential pressure, this is not always the case. When the fluid is at rest \((h = 0)\), it possesses gravitational potential energy \(P = \rho gz\) if \(z > 0\), known as hydrostatic fluid pressure. This suggests no gradient within hydraulic head and therefore no flow in accordance to Darcy’s Law. By running through the same
train of thought, \( h \) increases with depth if the fluid pressure is less than hydrostatic pressure which corresponds to upwelling flow. In the case of downwelling flow, fluid movement is counter-intuitive as low pressure fluids are guided towards the higher fluid pressure domain, indicating that the actual driving force is from the gradients of hydraulic head.

Darcy’s Law hence can be re-expressed by substituting hydraulic head (Eqn 2.3) into the original equation (Eqn 2.1 and Eqn 2.4). This revises the interpretation of \( u \) and is in line with physical diffusive equations.

\[
h = \frac{P}{\rho g} - z \tag{2.3}
\]

\[
q = \frac{k}{\mu} \left( \nabla P + \rho g \nabla z \right) \tag{2.4}
\]

Another type of flow that precedes gravity driven flow is buoyancy driven flow. Buoyancy driven flow is achieved via the change in fluid density due to thermal or chemical density gradients (Turcotte and Schubert 1982). This type of flow lead to the creation of convection cells. Flow rates in convection cells may approach 0.1 m.yr\(^{-1}\) and the occurrence of convective cells is controlled by the thickness of the aquifer, fluid-density gradient and regional permeability (Garven and Raffensperger 1997). Buoyancy driven flow can be further perturbed by a secondary heat source such as as pluton (Eldursi et al. 2009), leading to the rise of an intense secondary order fluid-flow within a slower regional fluid flow (Stern et al. 1992[97]).

The last type of flow relevant to this dissertation is deformation-driven flow. This is characterised by the change in permeability as a result from rock deformation (e.g. Thébaud and Rey 2013, Gessner 2009, Micklethwaite and Cox 2004, Cox 2001). Deformation-driven flow is derived from the propagation and healing of fractures leading to the formation of dynamic permeability. Previous experimental studies attempted to quantify the relationship of stress
and permeability for different type of rocks (e.g. Morrow et al. 2015[68], Wang and Park 2002[115], Brace et al. 1980[9]) while achieving a similar conclusion of permeability decay with increasing confining pressure. They had determined that pore size and permeability undergo at least five phases before the resultant collapse of the sample. The first phase is associated with the initial increase in cracks, enhancing porosity and permeability under increasing confining pressure. As confining pressure continues to increase, the newly developed cracks begin to contract, effectively reducing permeability and porosity. This marks the second phase of the experiment. In the third phase, the breakage of individual sandstone grains, leads to a slight increase in permeability and porosity. This increase in permeability continues to increase and in the fourth phase, it reaches an undefined peak permeability. The last phase occurs when those same cracks within grains start to contract, drastically reducing permeability and to the eventual collapse of the sample. The cycles of permeability from crack formation/sealing indicates the highly variable changes in permeability at increasing confining pressure. However, recent research has also determined that rocks are capable of decreasing permeability as soon as deformation occur (e.g. Micklethwaite et al. [65]). This suggests that the changes in permeability are time-sensitive. Strain-rate was chosen to assume the plastic deformation of rocks, capable of increasing and decreasing permeability in short periods of time. Establishing a new relationship with strain-rate to monitor the highly variable changes in permeability will be considered in this dissertation.

2.2.3 Conservation of Fluid and Energy

An account of the mass of fluid is require when simulating fluid flow. Consider a rectangular box with the dimensions of $x$ as the horizontal extent and $z$ as the box’s vertical extent. This rectangular box also represents an infinitesimal cell within each simulation (see Fig 2.1). The fluid flowing from the $x$ axis is $u$ and fluid flowing from the $z$ axis will be known as $v$. Flow flux at the $x$ axis is expressed as $u(\delta x) = u + \frac{\partial u}{\partial x} \delta x$. Likewise for flow flux at the $z$
axis is expressed as $v(\delta z) = v + \frac{\partial v}{\partial z} \delta z$. Fluid input takes place at two known sides. The two remaining sides are used to account for fluid flowing out of the box. The net flux out of the box is expressed as, for $x$ axis, $u + \frac{\partial u}{\partial z} \delta x$, for $z$ axis, $v + \frac{\partial v}{\partial z} \delta z$.

To determine the net rate at which fluid flows out of the box, the expressions need to be combined together in two dimensions. The outward flow rate in the $x$ axis is $\frac{\delta u}{\delta z} \delta x$ is multiplied by the area of the face across which the flow occurs, $\delta z$. This is likewise to flow in the $z$ axis where $\frac{\delta v}{\delta z} \delta z$ is multiplied by $\delta x$. The net outflow rate in the $x$ direction is thus
\frac{\delta u}{\delta x} \delta x \cdot \delta z. Similarly the net outflow rate in the z direction is \frac{\delta v}{\delta z} \delta z \cdot \delta x. The total outward fluid flux per unit area of the box is therefore:

\frac{\delta u}{\delta x} + \frac{\delta v}{\delta z} \cdot \delta z \cdot \delta x \cdot \delta z \cdot \delta x. \cdot \delta z.

If the flow is constant and there are no density variations to consider, the net flow in and out of the box equates to zero. Many numerical codes (including SHEMAT that is used in this study) rely on this assumption to characterise fluid flow. The assumption for an incompressible fluid (assuming the characteristics of an ideal fluid) simplifies the approach for mass conservation which is expressed as:

\frac{\delta u}{\delta x} + \frac{\delta v}{\delta z} = 0 \quad \text{(2.6)}

While the volume of fluid is being accounted for, the fluid also possesses a suite of hydraulic forces. These forces are identified as fluid pressure, fluid viscosity and gravity. Inertial forces of the liquid are disregarded as their influences over the overall acceleration of the fluid are minimal at the considered low velocities. This condition is held true in highly viscous fluids such as the Earth’s mantle where fluid movement is measured according to geologic timescales. The condition is also held true as it conforms to the second Newtonian law of motion, upholding the energy balance in the simulation.

The first force accounted for here is fluid pressure that occurs on four sides of the rectangular box. As pressure is force per unit area, the total force on each side (x,z) of the infinitesimal cell is \( p \delta \chi \cdot \delta z \). \( P_1(x) \) and \( P_2(x) \) represent opposite sides of the cell in the x direction. Therefore, the net pressure on the infinitesimal cell can be expressed in the x direction per unit area of the cell:

\frac{p_1(x) \delta z - p_2(x) \delta z}{\delta x \delta z} = \frac{[p_2(x) - p_1(x) \delta x]}{\delta x} = -\frac{\delta p}{\delta x} \quad \text{(2.7)}
Chapter 2

If the forces on the left and right side of Eqn 2.7 are equal, the pressure forces will cancel each other. Similarly, if we are to account the pressure forces on the z direction, the net pressure will become \(-\frac{\delta p}{\delta z}\).

The second force to consider is gravitational force. This is evaluated by the product of the fluid’s mass and acceleration due to gravity. In 2D geological modelling, gravity acts in the positive z direction. Therefore, the net gravitational force on the cell in the z direction is \(\rho g\).

The last force is fluid viscosity, which defines the fluid’s inherent resistance to movement. On the infinitesimal rectangular cell, these forces are found parallel and perpendicular to the cell’s surface. \(\tau_{xz}\) and \(\tau_{zx}\) representing viscous shear stresses. These are viscous force per unit area acting parallel to the surface of the cell. \(\tau_{xx}\) and \(\tau_{zz}\) represent viscous normal forces, which are the viscous forces per unit area acting perpendicular to the surface of the cell. If \(\tau_{xz} = \tau_{zx} = 0\), the net torque at the centre of the cell is null. Subsequently if the viscous normal forces are equal, there will be no torque. The net viscous force in the x direction per unit cross-sectional area of the block as the sum of the differences of the viscous forces, expressed as:

\[
\frac{\tau_{xx}(\delta x)\delta z - \tau_{xx}(\delta x)\delta z}{\delta z} + \frac{\tau_{zx}(\delta z)\delta x - \tau_{zx}(\delta z)\delta z}{\delta z} = \frac{\delta \tau_{xx}}{\delta x} + \frac{\delta \tau_{zx}}{\delta z} \tag{2.8}
\]

Similarly, the net viscous force in the z direction per unit cross-sectional area of the cell is: \(\frac{\delta \tau_{xz}}{\delta z} + \frac{\delta \tau_{zx}}{\delta x}\). In an ideal Newtonian viscous fluid, the viscous stresses are linearly proportional to the velocity gradients. The shear stress in any location in two dimensions yield, where \(u\) and \(v\) are horizontal and vertical components of fluid flow:

\[
\tau_{xx} = 2\mu \frac{\delta u}{\delta x}, \quad \tau_{zz} = 2\mu \frac{\delta v}{\delta z}, \quad \tau_{zx} = \tau_{xz} = \mu \left( \frac{\delta u}{\delta z} + \frac{\delta v}{\delta x} \right) \tag{2.9}
\]
Eqn 2.9 is then used to calculate the cell’s total normal stress.

\[ \sigma_{xx} = p - \tau_{xx} = p - 2\mu \frac{\partial u}{\partial x}, \quad \sigma_{zz} = p - \tau_{zz} = p - 2\mu \frac{\partial v}{\partial z} \] (2.10)

The negative signs in front of \( \tau_{xx} \) and \( \tau_{zz} \) are the result of the opposite sign conventions adopted for \( \sigma \) and \( \tau \). Viscous stress is the only contributor to shear stress. The viscous forces from Eqn 2.9 and Eqn 2.6 are re-expressed for the respective axes:

\[ \frac{\partial^2 v}{\partial x \partial z} = -\frac{\partial^2 u}{\partial x^2}, \quad \frac{\partial^2 u}{\partial z \partial x} = -\frac{\partial^2 v}{\partial y^2} \] (2.11)

\[ x = \mu \left( \frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} \right), \quad z = \mu \left( \frac{\partial^2 v}{\partial x^2} + \frac{\partial^2 v}{\partial y^2} \right) \] (2.12)

Using Eqn 2.11 for the mix partial derivatives, we arrive at Eqn 2.12 to account for the net viscous forces per unit cross-sectional area in their respective directions.

At this stage, it is now possible to assemble the force balance equations to account for fluid pressure Eqn 2.7, gravitational effect (\( \rho g \)) and viscous forces Eqn 2.12 to their respective axes. For the x-direction:

\[ 0 = -\frac{\partial p}{\partial x} + \mu \left( \frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} \right) \] (2.13)

And, for the z direction where gravitational force is applied:

\[ 0 = -\frac{\partial p}{\partial z} + \rho g + \mu \left( \frac{\partial^2 v}{\partial x^2} + \frac{\partial^2 v}{\partial z^2} \right) \] (2.14)

As fluids are given a constant hydrostatic pressure variation, \( P = p - \rho gz \) is introduced into Eqn 2.13 and Eqn 2.14 yielding the final equations at their respective axes.

\[ 0 = -\frac{\partial P}{\partial x} + \mu \left( \frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} \right) \] (2.15)
\[ 0 = -\frac{\delta P}{\delta z} + \rho g + \mu \left( \frac{\delta^2 \nu}{\delta x^2} + \frac{\delta^2 \nu}{\delta z^2} \right) \]  

(2.16)

### 2.3 Thermal considerations

Macro Earth processes such as plate tectonics require vast amounts of energy to initiate crustal movement, mountain building and volcanism. The driving source of energy is heat from the interior of the earth. This energy is provided from the decay of radiogenic isotopes \(^{232}\text{U},^{235}\text{U},^{232}\text{Th},^{40}\text{K}\) as well as the cooling of the earth. The energy associated with earthquakes, mountain building and volcanism accounts only for 1% of the heat flow lost to the surface (Turcotte and Schubert 1982). Further heat loss derives from the transfer of heat converted into a directed motion by thermal convection, provided that all forms of heat are transmitted at depth into the fluids. The mantle is heated from the lower boundary, causing the material to be lighter, rising to the surface. Once the heated fluid reaches to the upper yet cooler thermal boundary, the material begins to cool and spread towards the sides of the boundary. Density starts to increase, invoking negative buoyancy instability to sink back to the lower thermal boundary. However, the thermal phenomenon requires the material to over its inherent viscous resistance to convect.

The most basic form of heat transfer is conduction, which occurs through a medium via the net effect of molecular collisions. It is a diffusive process wherein molecules transmit their kinetic energy to other molecules by colliding with them. Conductive heat flow can be described with a diffusive law, similar notation of Darcy’s Law and is expressed as (Fourier 1878):

\[ q = -K \frac{\delta T}{\delta z} \]  

(2.17)
The law implies that the rate of thermal energy is churned out by the product of the coefficient of thermal conductivity, \( K \), and the geothermal gradient of the system. This equation assumes that the system has an isothermal gradient. The negative sign indicates heat flowing in the direction of decreasing temperature. A positive \( \frac{\delta T}{\delta z} \) indicates a growth of temperature in the positive \( z \) direction, therefore heat must flow from the negative \( z \) direction. In non-isothermal systems, the geothermal gradient is also applied. When numerical techniques simulate heat processes, \( K \) is assumed to be constant.

The simulations used in this dissertation assume constant temperature at the horizontal boundaries, with an upper cooler thermal boundary (\( T \sim 20^\circ C \)) and a warmer lower thermal boundary (\( T \sim 800^\circ C \)). The fluids are assumed not to have any capability of generating their own heat source. Thus, their established temperature fields, adhering to macro Earth processes, drive the simulations. As the fluid is dependent on its energy state, a couple of criteria were applied to analytically describe fluid activity.

### 2.3.1 Rayleigh number

In the absence of convection, the temperature difference, \( \Delta T = T_1 - T_0 \), and a stationary fluid, it is assumed that the temperature field is in a conductive state. This will reflect the arbitrary small Darcian velocities present in the model. As \( \Delta T \) increases, the fluids continue to exhibit the same behaviour until \( \Delta T \) reaches a threshold value that signifies the overcoming of those internal viscous forces. Therefore, the onset of convection is nearly the conduction temperature profile and \( \Delta T \) would be arbitrary small.

\[
Ra = \frac{\rho_0 g \alpha_v (T_1 - T_2) L^3}{\mu \kappa} \quad (2.18)
\]

The dimensionless Rayleigh number (\( Ra \), Eqn 2.18) measures a system’s tendency to produce free convection, that is, fluid flow driven by density variations. \( Ra \) is evaluated on the ratio of buoyant forces, which is conducive for convective fluid flow against the internal
viscous forces that inhibit convective flow. The mathematical expression observes the fluid’s change of temperature, $\Delta T$, specific weight, $\rho g$, thermal expansion coefficient of the fluid, $\alpha_v$, the cube of the depth of the system, $L^3$, over the product of the fluid’s viscosity, $\mu$ and the thermal conductivity of the medium, $\kappa$. In a heterogeneous permeability simulation, the mean of $k$ is used instead to provide that first order approximation.

$Ra_{crit}$, which marks the onset of convection, was found to be $4\pi^2$ (Lapwood 1948). When $Ra < Ra_{crit}$, fluid disturbances will decay overtime; subsequently $Ra \geq Ra_{crit}$, perturbations will grow overtime. However, this value is sensitive to the simulation’s aspect ratio as $4\pi^2$ remains true when the simulation’s aspect ratio is 1.0. With different aspect ratios, $Ra_{crit}$ can be evaluated by $Ra = \pi^2 \min(b + \frac{1}{p})^2$ where $b = \sqrt{(pA_x)^2 + (qA_y)^2}$ (Beck 1972). $A_x$ and $A_y$ are the ratios of the model’s depth and length of the axis $(x, y)$. Non-negative integers $p$ and $q$ function as the on-off switch for 2D and 3D models. As this dissertation deals with 2D simulations, $p$ was set to 1 and $q$ was set to 0. This new evaluation does not affect the interpretation of $Ra$. However, it is important to note that $Ra_{crit}$ was evaluated under the assumption that the model has fixed thermal boundaries and homogeneous media.

In this study, as the simulations assume models of homogeneous materials in a dynamic permeability field, the evaluated $Ra_{crit}$ does not fulfill the conditions to determine fluid instability. One possible solution is to use a criterion that splits the model into smaller blocks (Simmons et al. 2010, Nield and Simmons 2007). The method utilises the means of physical properties (such as permeability and heat capacity) to compute $Ra$. If $Ra > Ra_{crit}$ at any of these blocks, fluid instability is present in the model. Analytical work on the Horton-Rogers-Lapwood model has expanded on potential $Ra_{crit}$ based on different boundary conditions, as seen in Table 2.1. $K$ and $L$ represents media’s permeability and the horizontal dimension of the media, respectively. The subscripts $l$ and $u$ indicate the horizontal and the vertical dimensions of the model. Because $Ra_{crit}$ changes according to simulations’ aspect ratios and boundary conditions, pursuing this is out of the scope of the project. However, to remain true
Table 2.1 Values of Critical Rayleigh number $Ra_c$, and the corresponding critical wavenumber $\alpha_c$ for various boundary conditions (after Nield (1968)). The terms free, conducting, and insulating are equivalent to constant pressure, constant temperature, and constant heat flux, respectively. Modified from Nield and Bejan (2006) Table 6.1

<table>
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<th>IMP</th>
<th>CON</th>
<th>CON</th>
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<th>$\alpha_c$</th>
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<td>IMP</td>
<td>CON</td>
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<td>0.00</td>
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</tr>
</tbody>
</table>

Table 2.1 Values of Critical Rayleigh number $Ra_c$, and the corresponding critical wavenumber $\alpha_c$ for various boundary conditions (after Nield (1968)). The terms free, conducting, and insulating are equivalent to constant pressure, constant temperature, and constant heat flux, respectively. Modified from Nield and Bejan (2006) Table 6.1

To the literature, this dissertation will use the threshold value of $Ra \approx 39.48$ (Lapwood 1948). The use of the evaluated $Ra_{crit}$ (Beck 1972) is applicable when the simulation has either met the conditions or when convection cells can be seen during analysis.

### 2.3.2 Peclet Number

The dimensionless Peclet number, $Pe$ is commonly used within numerical simulators such as SHEMAT to estimate the relative dominance of the heat transport mechanism with a given length scale.

$$Pe = \frac{\rho c \bar{u} R}{k} \quad (2.19)$$

$Pe$ is expressed by the relation of fluid flow through an aquifer, a ratio of the product of the mean of Darcy’s velocity, $\bar{u}$, fluid density, $\rho$, characteristic length of the process, $R$, heat capacity of fluid, $c$ over the intrinsic permeability of the medium. The critical value of $Pe$ is 1. For $Pe < 1$, diffusive heat transport becomes more dominant than advective heat
transport. For values more than 1, the influence of heat transported via advection dominates at the analysed location. At higher Peclet numbers, advective heat transport dominates.

2.3.3 Energy Budget

In a broader Earth system, heat from the mantle transfers its energy via conduction to the crust. At micro scale, we look into the individual cells that make up the model. Heat goes in one direction and escapes by another direction. This requirement is illustrated in the same rectangular block (Fig 2.1) with $\delta x$ and $\delta z$ as their respective axes. Heat flux in the $x$ direction is $q_x$ whereas it is $q_z$ in the $z$ direction. The rate of heat flowing into the box in the $z$ direction is $q_z(z)\delta x$. Similarly the heat flux moving in from the $x$ direction is $q_x(x)\delta z$. The heat flow rates flowing out of the cell in $z$ direction is $q_z(\delta z)\delta x$. Likewise for the heat flow flowing out of the cell in the $x$ direction is $q_x(\delta x)\delta z$. It is now possible to determine the net heat flux out of the system:

$$\{q_x(x + \delta x) - q_x(x)\}\delta y + \{q_z(z + \delta z) - q_z(z)\}\delta x = (\frac{\delta q_x}{\delta x} + \frac{\delta q_y}{\delta y})\delta x\delta y \quad (2.20)$$

$$\frac{\delta q_x}{\delta x} + \frac{\delta q_z}{\delta z} = \rho H \quad (2.21)$$

In steady state, the right size of Eqn 2.20 requires to be greater than zero, which suggests internal heat generation by the block. This internal heat flux is expressed as $\rho H(\delta x\delta z)$ causing Eqn 2.20 into Eqn 2.21.

Heat flux evaluated from Eqn 2.17 is applied to any direction to the temperature gradient. By making $K$ constant, Eqn 2.17 is rewritten as:

$$q_x = -K\frac{\delta T}{\delta x}, \quad q_z = -K\frac{\delta T}{\delta z} \quad (2.22)$$
Eqn 2.22 is then substituted into Eqn 2.21 to obtain

\[-k \left( \frac{\delta^2 T}{\delta x^2} + \frac{\delta^2 T}{\delta z^2} \right) = \rho H \]  

(2.23)

If fluid or the medium is not capable of generating any heat, Eqn 2.23 will instead equate to 0. This form is known as Laplace’s equation.

When the fluid is heated, the fluid’s density decreases as a result of its thermal expansion. Boussinesq approximation accounts for the energy created by these density variations. However, these forces from density variations are found to be applicable at temperatures less than 28° C (Gray [39]). The simulations presented in this dissertation are with temperatures up to 800° C, which is over the limit set by Gray (1976). The Boussinesq approximation will not be considered.

2.4 Permeability and its estimation

Permeability controls the mobility of fluids through the interconnected pore space of a porous medium (Cathles and Adams 2005). A meaningful estimation of permeability is essential to determine the feasibility of important geologic processes such as advective solute transport, advective heat transport, and the generation of elevated fluid pressures (Cathles and Adams 2005). Permeability used in this dissertation is considered as intrinsic permeability, a property of the medium at standard temperature and pressure (Ingebritsen and Manning 1999).

Permeability estimation is challenging because of its inherent variability over 12 orders of magnitude and time-sensitive deformation can alter their permeability values, seen in Fig 2.2. The precipitation and dissolution of minerals do have an effect that spans at least 5 orders of magnitude (Rutqvist and Stephansson 2003). Furthermore, during tectonic processes, the permeability is expected to change at each time-step. This is conceptualised as ’Dynamic
permeability’ to describe this time-sensitive process (Cathles and Adams 2005). However, the means to monitor and apply minute changes to permeability have not been attempted. Therefore, this dissertation attempts to account for the time-induced deformation through the implementation of strain-rate as a conservative first-order approximation to dynamic permeability (Chapter 4).

In order to include strain-rate, generating a base anisotropic permeability is essential. Laboratory experimental results have confirmed the trend of permeability decay when depth increases (e.g. Brace et al. 1968, Rutqvist and Stephansson 2003 and Morrow et al. 2014). By extrapolating these results, three permeability-depth decay curves were developed, seen in Eqn 2.3. This dissertation will settle on the permeability-depth equation by Ingebritsen and Manning (1999) for its successful record on crustal-scale fluid flow and is compatible with other compiled data (e.g. Shmonov 2003, Stober and Bucher 2007) and its representation for deep crust in stable cratons (Ingebritsen and Manning 2010[49]). Although the other curves were derived from experimental data, the permeability-depth function (Ingebritsen and Manning 1999) covers a wider range of rocks, thus making suitable for any regional study.

2.5 Fluid Simulation in SHEMAT

In this work, the fundamental transport equations are solved with the Simulator of Heat and Mass Transport (SHEMAT), a finite difference simulation code which is able to solve complex models and simulate coupled heat in fluid scenarios (Clauser 2003). SHEMAT is able to simulate fluids in full 3D geological models. The code was applied to low-temperature simulations in geothermal and mineral systems (e.g. Zhao et al. 2002, Gessner 2009, Kuhn and Gessner 2009[58]).

SHEMAT has also been augmented with PySHEMAT (Wellmann et al. 2012) as a means to automate the creation of a multitude of models of different parameters. The script allows
Fig. 2.2 Permeability measured in fractured crystalline rocks at Gidea, Sweden (data points from Wladis et al. (1997). Effects of shear dislocation and mineral precipitation/dissolution processes overwrite the dependency of permeability at depth (stress). The permeability values on the left-hand side represent intact granite, whereas the permeability values on the right-hand side represent highly conductive fractures. Taken from Rutqvist and Stephansson (2003[85]).

Fig. 2.3 Comparison of permeability-depth decay functions (Manning and Ingrebitsen 1999[51], blue line), Experimental (Shmonov et al. 2003[90], green line) and Black Forest (Stober and Bucher 2007[98], red line).
a seamless transfer of information (i.e. geology, temperature field and strain-rate) through the use of arrays into SHEMAT. SHEMAT contributes the fluid flow simulations from a single time-step extracted from another non-fluid process simulator, such as data temperature, strain-rate and geology from Ellipsis3D (Chapter 4).

2.5.1 Governing equations

SHEMAT solves the relevant equations that simulate fluid flow and heat transfer. Under a confined aquifer setting, it combines Darcy’s Law (Eqn 2.1) and the conservation of mass (Eqn 2.15, Eqn 2.16), hydraulic constant density reference potential \( h_0, h_0 = z + \frac{P}{\rho_0 g} \) and an account of the change of fluid pressure through time, \( \frac{\partial P}{\partial t} = \rho_0 g \frac{\partial h_0}{\partial t} \), to create the groundwater transport equation (Eqn 2.24). In order to yield the solutions in Cartesian coordinates, the divergence of Eqn 2.24 is taken for each axis.

\[
\rho_f g (\alpha + \phi \beta) \frac{\partial h_0}{\partial t} = \nabla \left[ \frac{\rho_f g k}{\mu} (\nabla P + \rho_f g \nabla z) \right] \tag{2.24}
\]

Heat transfer is evaluated with the change of heat content of a control volume, \( dV \), with surface area, \( dF \), during a time interval, \( dt \). Conservation of energy requires that the change of heat in time equals to the transfer of heat (diffusion, advection) and the production of heat (Eqn 2.25), where \( \mathbf{n} \) is the unit vector associated with the surface \( F \), perpendicular to \( F \) and directed outward.

\[
\int_v \frac{\partial Q}{\partial t} dV = \int_v \frac{\partial}{\partial t} (\rho c T) dV = \int_F (\lambda \nabla T - \rho_f c_f T v) \mathbf{n} dF + \int_V H dV \tag{2.25}
\]

Thus, a single control volume \( dV \) is given which is then expanded to solve in Cartesian coordinates for the SHEMAT block.

\[
\frac{\partial Q}{\partial t} = \frac{\partial}{\partial t} (\rho c T) = \nabla (\lambda \nabla T - \rho_f c_f T v) + H \tag{2.26}
\]
2.5.2 Finite Difference Method

SHEMAT computes the solutions by using a block centred finite difference method. The method uses the discretization of the derivative of the generic differential equation, \( y'(x) = \frac{dy}{dx} = \lim_{\Delta x \to 0} \left( \frac{y(x+\Delta x) - y(x)}{\Delta x} \right) \). Instead of describing the differential \( dy/dx \) by limited \( \Delta x \), a finite value of \( \Delta x \) will be used. This expression applies to a forward finite difference method. SHEMAT on the other hand considers the difference from the cell before, \( y(x - \Delta x) \), and the cell after, \( y(x + \Delta x) \) to determine an approximate result with respect to the function.

The setup of a SHEMAT model uses a block-centred grid, where nodes are located at the centre of the grid cells. With K0 at the top of the grid representing the vertical aspect (top to bottom), \( i \) represents the horizontal aspect (left to right), and \( j \) represents the diagonal aspect (front to back).

The architecture of the model is based on a rectangular domain that has been subdivided into smaller rectangular blocks. Each block identified by the grid SHEMAT contains the values of the assigned properties. Each block is identified by their grid indices and is separated by grid lines (Zheng and Bennett [127]). All governing equations are solved at each block in a series of approximating differentials in a prognostic partial differential equation (Clauser [14]). The result of this discretization provides a systematic way of solving linear finite difference equations via a numerical method. The finite difference method is not without disadvantages as the evaluations are only approximations and often cause instability (Stuwe [99]). For SHEMAT, it uses two criteria to overcome these limitations.

The Courant criterion ensures the continuity of the conversation of mass at each time-step (Clauser [14]). The Courant criterion is expressed as the ratio of fluid velocity flowing into the cell over time-steps, \( v \cdot \Delta t \) and the amount of void spaces in the same aspect, \( \phi \cdot \Delta x \). The criterion is expanded to other dimensions. SHEMAT considers Courant criterion \( \leq 1.0 \) for the simulation to remain stable.
Chapter 2

The Neumann criterion handles the conservation of energy in the simulation. It prevents the conductive thermal gradient from inverting in the course of the simulation (Clauser [14]). This criterion is expressed as the ratio of fluid thermal conductivity and time-steps, \( \lambda \cdot \Delta t \), over the cell’s thermal capacity, \( \rho \cdot c(\Delta x)^2 \). Similar to the Courant criterion, the Neumann criterion is expanded to include model’s other dimensions. SHEMAT considers Neumann criterion \( \leq 0.5 \) for the simulation to remain stable. At higher Courant or Neumann values, the possibility of computing numerical errors increases. There are two possible ways of reducing numerical error.

2.6 Chapter Summary

An overview of the theoretical considerations pertaining to fluid flow and heat transfer in geological systems was presented in this chapter. Much analytical work was done to uncover the limitations of Darcy’s Law and the evaluation of the conservation of mass and energy in numerical models. The chapter also touched on the problems in estimating intrinsic permeability encountered in this dissertation. Numerical codes such as SHEMAT was introduced with its governing equations.
Chapter 3

Fluid flow and Mineralising patterns in Benchmark simulations

3.1 Preamble

Gold ore forming processes are associated with heat, fluid and metal transfer within the crust. Recent developments of numerical tools provide unique opportunities to simulate and then evaluate the physical parameters associated with Au mineralisation (e.g. Mt Isa Copper deposit by Kuhn and Gessner 2009, New Guinea by Gow et al. 2002 and Golden Mile by Hobbs et al. 2000. Amongst the physical parameters associated with mineralisation, the interplay of thermal gradient and rock permeability form a first order control on where mineralisation may occur when the crust undergoes deformation (Nield and Bejan 2006, Phillips 1991). Rock permeability is commonly assumed to be isotropic and homogeneous in numerical modelling. However, rock permeability values from geological rock records have been found to range over 10 orders of magnitude and to be the dominant factor for driving crustal fluid flow (Kuhn and Gessner 2009). The geothermal field is also an important constraint as it provides the necessary energy conditions for density driven flow. While such permeability conditions may be sufficient, the fluids may not have the means to undergo
advection if there is sufficient energy from the geothermal gradient. Similarly, advective flow will not take place in domains associated with significant geothermal gradients and low permeability fields (e.g. $< 1.0^{-18}$ m$^2$). This chapter evaluates the conditions required for the formation of hydrothermal convective cells within a generic Precambrian granite-greenstone model through an expansion of a known alteration index equation and a fluid flow numerical simulator.

### 3.2 SHEMAT Modelling Approach

The simulations were conducted with a known fluid flow simulator, SHEMAT, to observe fluid flow in a single time-step of a tectonic evolution of a given terrane. SHEMAT is a coupled fluid, heat and reactive transport simulation code (Clauser 2003) that had been widely applied to simulations in low-temperature geothermal and mineral systems (e.g. Gessner 2006, Kuhn and Gessner 2009, Kuhn and Stofen 2005). SHEMAT contributes to the fluid flow process from single time-step extracted from other non-fluid flow numerical codes (such as Ellipsis) as inputs. SHEMAT assumes that the simulation contains an infinite supply of fluids available from the bottom and is already saturated by fluids. Initial hydraulic head is set at 8,000 m, assuming the datum is the vertical extent of the model.

#### 3.2.1 Model Conditions

Gold mineral systems form during major episodes of juvenile continental crust formation and crustal anatexis throughout the earth history (Goldfarb et al. 2001). Major Au endowment was formed at specific times during Archean and Proterozoic eons and it was hosted in greenstone belts surrounded by granitoids (Goldfarb et al. 2001). Many gold deposits occurring within the granite-greenstone terranes show a close spatial association with granitic plutons. However, the precise role of these intrusions in ore formation is often debated.
Some models suggest that the granitoids are at least one source of ore-fluids and solutes (e.g. Doublier et al. 2014). Others suggest that granitoids exert an important structural control on gold mineralization (e.g. Groves et al. 2003). Still others suggest that granitoid provides the heat engine that empowers hydrothermal fluid circulation associated with mineralisation (e.g. Thébaud and Rey 2013).

In order to test the latter hypothesis, we present a series of models that shows a generalized setting through Models 1 to Models 4 (M1 to M4), mimicking granite-greenstone terranes under different permeability and geometry fields. Each model will use a simplified bimodal lithological setting, greenstones and granites with the exception of M1 and M2. M1 and M2 simulations represent modified benchmark models from Elder (1967) and consist of greenstones under different permeability conditions. Simulations M3, M3V, M4 and M4V contain greenstones and are envisaged as vertical cylinders or channels, following a valid assumption as suggested by gravity surveys conducted in the Pilbara craton (Drummond 1983). The aspect ratios (ratio of length and depth of model) for all simulations are kept at 0.8 in order to replicate those shown in Elder (1967). The discretization size for each simulation is kept at 250 m, providing a matrix of 1,280 cells. The fluid boundaries for all models are kept as impermeable, to be consistent to the Elder (1967) model.

As the original thermal conditions were not specified in the original Elder (1967) model, a temperature field needed to be generated. The temperature field was generated within a generic granite-greenstone terrane thermo-mechanical model in Ellipsis, a Lagrangian integration point finite element code that is capable of tracking time dependent variables in a Eulerian mesh (Moresi et al. 2002, 2001). By setting a constant basal heat flux of 0.025 W.m$^{-2}$, a temperature field was generated with a lower temperature limit of 20.2$^\circ$ C and an upper temperature limit of 171.4$^\circ$ C. The temperature field was then transferred into the SHEMAT model, creating a upper thermal boundary of 20.2$^\circ$ C and a lower thermal boundary at $\sim$ 171.4$^\circ$ C.
Fig. 3.1 Permeability fields and their geometries for generalised models (M1 to M4). M1 represent the benchmark model from Elder (1967) for fluid flow simulations utilising a homogenous and isotropic permeability field. M2 is a modified model from Elder (1967) to illustrate a variable permeability field evaluated from Ingebritsen and Manning (1999) permeability-depth equation. M3 and M4 implement the ‘channel-like’ higher permeability fields. Dimensions of channels are different for M3, M4 and their variable variants. The permeability fields for M3V and M4V are evaluated from the permeability-depth equation while keeping the granite’s permeability at $10^{-18}$ m$^2$. 
The generalized simulations (M1 to M4) have permeability fields of increasing complexity (Fig 3.1) and fluid flow will be assessed within the greenstones. These greenstones were assigned a rock permeability ranging from $k = 10^{-12.0}$ to $10^{-19}$ m$^2$ whereas the granites were assumed to be impermeable, with an intrinsic isotropic permeability of $k = 10^{-18}$ m$^2$. In a lode-gold or orogenic gold system, granites were found to be heat engines for encouraging fluid flow via regional or contact metamorphism (e.g. Groves et al. 2003). Setting granites impermeable further aided in studying fluid flow within the greenstones packages. The thermal conductivity of greenstones, $\lambda_{gs}$, were assigned with 2.559 W.m$^{-1}$.K$^{-1}$ and its specific heat capacity, $c_{gs}$, was assigned as 1000 J.kg$^{-1}$.K$^{-1}$. The thermal conductivity of granites, $\lambda_{gr}$, were assigned with 2.448 W.m$^{-1}$.K$^{-1}$ and its specific heat capacity, $c_{gr}$, were assigned as 1000 J.kg$^{-1}$.K$^{-1}$. These conservative thermal conductivity values represent the lower end members of the wide spectrum of values presented in Stuwe (2007). Greenstones and granites have similar heat capacities of 800 J.kg$^{-1}$.K$^{-1}$ (Stuwe 2007) however, we assigned the rocks a slightly higher specific heat capacity to maintain that similar ratio as presented in the literature. The porosity values for both rocks were set at 1%, which is towards the lower-end of acceptable values for SHEMAT (Clauser 2003).

The estimation of rock permeability in any geologic model is a requirement for any fluid flow calculations. In this chapter, the evaluation of the permeability field is derived from the permeability-depth equation. The rocks were assumed to be in a metamorphic setting with rock permeability, $k$ (m$^2$) undergoing a quasi-exponential decay according to depth, $z$ (km), which is captured in $\log k = -14 - 3.21 \log z$ (Ingebritsen and Manning 1999).

The geometry of each permeability field differs in each generalized simulation (Fig 3.1). An isotropic permeability field was assigned for M1 benchmark model, which is kept at $k = 10^{-14}$ m$^2$. The variable permeability field for M2 benchmark model was evaluated by a permeability-decay curve (Ingebritsen and Manning 1999). In M3 and M4 simulations, a bimodal permeability field was applied, with permeability fields resembling ‘channels’ of
different geometries similar to greenstones as vertical cylinders. The greenstone channel extends vertically for 3 km from a defined thickness of greenstone cover (2 km). The width of the greenstone channel in M3 was set at 2.5 km, mimicking a greenstone keel. M4’s greenstone channel width was decreased to 1 km to accommodate at least three of such channels in the domain. The permeability fields for the greenstone channels were computed from the permeability-depth equation function (Ingebristen and Manning 1999).

Each model is simulated for 100 time-steps of 1,000 years each with 50 iterations to ensure numerical stability. The outputs are checked from the 25th, 50th and 75th time-step to check to ensure steady-state has been achieved.

3.2.2 Numerical Mineral Potential Analysis

In addition to conducting a fluid flow analysis, simulations results were post-processed using the rock alteration index (RAI) (e.g. Phillips 1991) in order to evaluate the mineralization potential for Au. Initially published as IRAI from Zhao et al. (2000), the method utilises the equation given as the RAI. Mineralising patterns can be deduced from the product of geothermal gradient, $\nabla T$ ($^\circ$C/km), and fluid velocity, $u$ (m.s$^{-1}$), by using RAI (Phillips 1991). The RAI has been used and modified in previous work such as the isolation of movement of fluids empowered by a plutonic emplacement (Eldursi 2009) and the determination of mineralising patterns in different model geometries (Zhao 1998).

Hydrothermal fluids contain dissolved chemical species that flow through geologic media. In many geologic environments, reactants in solution can be delivered to the reaction site by advection and diffusion. The dissolution/precipitation of an aqueous mineral via advective processes overpowers diffusive processes when large-scale processes (i.e. fluid circulation over a large time scale) are considered (Wood and Hewett 1982).

The Péclet number, $Pe$, was used to measure the relative dominant process that transported given chemical species in the simulation. $Pe$ is a dimensionless number used in SHEMAT.
as a numerical criterion for the processes of convective heat exchange. The number $Pe$ characterises the relationship between advective and conductive heat transport, where the product of depth of the model, $l$ (m) and fluid velocity, $u$ (m.s$^{-2}$) over the ratio of permeability (m$^2$) and the product of density, (kg.m$^{-3}$) and the thermal capacity of the porous medium, $c_p$ (m$^2$.kg.s$^{-2}$.K$^{-1}$) (Turcotte and Schubert). At higher $Pe$ values ($Pe > 2$), advective heat exchanges are more dominant in the model.

RAI can be expanded into $RAI_{Au}$ to identify probable precipitation and dissolution region of a specific mineral (in this case, Au, as indicated in subscript) of a hydrothermal system (Zhao) shown below. In these 2D simulations, it was found that $RAI_{Au}$ occurs in the lateral dimension. In addition, fluid driven by regional or contact metamorphism predicted to have Darcian velocities from $10^{-8}$ to $10^{-11}$ m.s$^{-1}$ (Ferry et al. 1992, Cook et al. 1997, Gerdes et al. 1998). $RAI_{Au}$ will also be using a conservative range from $10^{-8}$ to $10^{-10}$ m.s$^{-1}$ to isolate any potential mineralisation influenced by metamorphic driven fluid flow.

$$RAI_{Au} = \frac{\partial C_e}{\partial T} (\overrightarrow{u} \cdot \nabla T)$$  \hspace{1cm} (3.1)

Gold occurrences are common within Archean granite-greenstone terranes such as the Yilgarn, Superior and the Pilbara craton. The nature of ore fluids and proposed metamorphic models for these terranes is largely interpreted to carry Au as reduced sulphur complexes, for example, H\text{Au(HS)}$_2$. These sulphur complexes were also found within banded iron-formations (Phillips et al. 1984), as a result of suphidation of Fe-rich host rocks and a syn-deposition of Fe sulphides and Au. The presence of these sulphur complexes is largely associated to a pyrite-prrhotite buffer system and it is suitable for a first order approximation of Au solubility. Therefore, in these generalised granite-greenstone simulations, the nature of the hydrothermal fluid present is assumed to be a pyrite-pyrhhotite buffer system (Shenberger and Barnes 1989). Au’s respective solubility with respect to temperature is expressed in the piecewise equation below.
Hence, the aim for each simulation is to determine key fluid movements in generalised geometries. Each simulation underwent the workflow to evaluate specific conditions for mineralisation potential based on \( RAI_{Au} \) values.

\[
\log C_{Au}^e = \begin{cases} 
0.0369T - 7.1845 & (0^\circ C \leq T < 50^\circ C) \\
0.03T - 6.84 & (50^\circ C \leq T < 100^\circ C) \\
0.0248T - 6.32 & (100^\circ C \leq T < 150^\circ C) \\
0.0208T - 5.72 & (150^\circ C \leq T < 200^\circ C) \\
0.0144T - 4.44 & (200^\circ C \leq T < 250^\circ C) \\
0.0096T - 3.24 & (250^\circ C \leq T < 300^\circ C) \\
0.0036T - 1.44 & (300^\circ C \leq T < 350^\circ C)
\end{cases}
\] (3.2)

3.3 Results and Discussion

The permeability simulations of increasing complexity (Fig 3.1) were assessed on their fluid flow and mineralisation potential based on the analysis of the RAI. Each simulation achieved steady-state conditions within the first 10 time-steps, the results presented in this section is the 80th time step to keep the analysis constant. Dimensionless numbers such as the Rayleigh number would analytically determine the occurrences of fluid convections if certain conditions are met.

3.3.1 M1 simulation

The M1 simulation was designed to reproduce the results from Elder (1967) simulations. M1 contained an isotropic and homogeneous permeability field (M1 in Fig 3.1), fulfilling the conditions to calculate the Rayleigh number (discussed in Chapter 2) that determines occurrences of fluid convection. \( Ra_{M1} \) was evaluated to be 102.02. This is much greater than the evaluated \( Ra_{crit} = 20.233 \). Advective flow dominance was established with a maximum
estimated $\text{Pe}_{M1}$ of 155.0. According to Beck (1972) at the current aspect ratio of 0.8, we expect to see one convection cell at steady-state conditions.

Fig 3.2 shows the fluid results for the M1 simulation. The fluid vectors (Fig 3.2 (A)) show fluid movement forming a single convective cell, as predicted in Beck (1972). Lower fluid fluxes occupy the lower regions of the model, whereas the higher fluid fluxes are observed at the upper half of the model. As fluids start to convect from the left side, the 40°C temperature contour was observed to be closer to the surface (1.25 km) as compared to the right side of the model (∼4.0 km). This resulted in a higher geothermal gradient in region 2 than in region 3. Fluid fluxes were increased as a result from an increase in buoyancy forces and a greater geothermal gradient. The fluid was then cooled by the upper cooler thermal boundary leading to a lower temperature contour shown at the right side (40°C at the depth of 3.75 km).

As fluid is heated from the bottom, fluid velocity increased as a result from the combination of gravity induced flow and a subsequent decrease in fluid density. Fluid velocity is observed to peak till the fluids breaches an arbitrary boundary separating low and high fluid fluxes. When the fluid crosses this flux-controlled boundary (shown above the 80°C temperature contour), fluid velocity drops significantly as a consequence to the restoration of initial density and influence of advective flow dominance. Fluid’s density is restored before sinking back to the bottom of the model, creating the convection current.

The regions suitable for possible mineralisation were found at the upper left-side and the lower-half portions of the model after the application of RAI, seen in Fig 3.2 (B). As $\text{RAI}_{\text{Au}}$ is evaluated as a function of fluid flux and temperature gradient, the regions show areas where the lateral thermal gradient is negative. Fluid heating (Fig 3.2 (B), (1)) which leads to positive lateral thermal gradient, is described as positive from the heating process. As soon as fluid leaves the region around (1), fluid starts to lose its energy and seen as negative lateral thermal gradients. This creates an area suitable for probable mineral precipitation.
Fluid is observed to move towards (2) which is described as a heating and cooling portion of the model. Heating is created from the influx of fluids moving from (1). However, at the same time, a portion of the area experience cooling. As fluids move towards (3), the fluids are cooled which is represented in a positive RAI values suggesting that the minerals are potentially mobilised. When referred to the 40°C temperature contour (Fig 3.2), the gradient is observed to be above zero. As fluids migrate to (4), a negative lateral thermal gradient was briefly observed before getting reheated from the lower thermal boundary.

Fig. 3.2 (A) shows yearly fluid flux plot with temperature contours and dimensionless infinitesimal fluid indicating fluid movement for M1 in steady-state conditions. The RAI map of M1 in steady-state conditions with infinitesimal fluid vectors showing potential areas of mineralization and dissolution (B). Colour bars below each figure display fluid flux per year (A) and relative potentials of probable precipitation of Au (negative, red) and probable dissolution of Au (positive, blue). Number yellow circles (1) to (4) refer to areas of discussion pertaining to convection currents and RAI interpretation.

The application of RAI indicates regions of inactivity. They are marked by white regions, notably at the top and some regions at the bottom. According to RAI, the thermal gradients recorded in these regions are zero. Since the model was extracted from the Ellipsis model, fluid analysis is confined within the boundaries of the greenstones. Therefore, based on the restrictions, the white boxes seen in Fig 3.2 (B) relate to the mantle unit. For the top row, a constant upper temperature boundary of 21.8°C was set and do not change. The presence
of the constant upper model temperature boundary can potentially cause boundary effect. Despite having a large model (8 km by 10 km) with a discretization size of 250 m, it is challenging to avoid boundary condition effects.

In summary, M1 is described as the benchmark model reproduced from Elder (1967) capable of producing a single convective cell. The application of $RAI_{Au}$ provided the means to monitor regions of positive and negative lateral thermal gradients. Negative lateral thermal gradients are found at the lower half of the convective cell whereas the positive lateral thermal gradients are observed to occupy the upper half of the convective cell.

### 3.3.2 M2 simulation

The M2 simulation contains a variable permeability evaluated from the permeability-decay curve (Ingebritsen and Manning 1999) as a modification to the Elder (1967) simulation. Unlike M1, the variable permeability did not fulfill the conditions required to calculate Rayleigh number. SHEMAT evaluated $Pe$ to achieve the maximum of 0.187, indicating diffusive flow dominance. The steady-state solution was instead to determine the possibility for fluid instability.

Fig 3.3 shows that the steady-state fluid flow results overlain by the temperature contour and fluid flux plots for M2 simulation. The thermal contours show a steady decrease in temperature from the base to the top, inferred from the equal spacing of each temperature contour. Fluid movement was observed to flow in an anticlockwise motion, creating two uneven convective cells. The streamline overlay in Fig 3.3 (B) confirms the presence of localized fluid circulation.

Fluid flux (Fig 3.3 (A)) is observed to form three velocity-related regions. At the bottom of Fig 3.3 (A) at (1), fluids have low fluid flux despite having the highest temperature ($> 140.0^\circ$ C). The permeability near the base was $k = 10^{-18}$ to $10^{-16}$ m$^2$, restricting fluid movement. Higher fluid flux of $2*10^{-12}$ m.s$^{-1}$ was observed at Fig 3.3 (A) (2) and is
Fig. 3.3 (A) shows fluid flux with temperature contour and dimensionless infinitesimal fluid vector overlay for M2 simulation. (1), (2) and (3) represent regions for further discussion. (B) shows the outcome of M2 simulation after the application of $RAI_{Au}$ and streamline flows at the surface, outlining localized fluid circulation. Colour bars below each subfigure display fluid flux (A) and relative potentials of probable precipitation of Au (negative, red) and probable dissolution of Au (positive, blue).

bounded in between the 140° C and the 100° C temperature contours. Higher fluid fluxes were produced due to the increase of permeability, removing the restrictions found in (1). Lateral fluid movement was observed with the downwelling at the left side and upwelling from the right side. Fluid movement at region (3) was similar to the fluid movement in region (2) but at reduced fluid velocity. Two concave features were observed from the movement of the fluids before undergoing circulation at the surface. The concave feature became more defined when closer to the surface. As the fluids flowed towards the surface of the model, it was cooled by the upper cooler thermal boundary to restore fluid density before sinking to the lower thermal boundary. The fluid’s behaviour exhibited an elliptical circulation motion suggesting a localised fluid circulation. However, the presence of the constant upper temperature inflicts a constant temperature boundary resulting to a possible numerical error. A higher discretization size or a change to model geometry might be needed to resolve these boundary effects.
The implementation of RAI shows two distinct areas for positive (positive RAI) and negative (negative RAI) lateral thermal gradients (Fig 3.3(B)). The region for negative lateral temperature gradient dominated the whole model except at the central lower portion of the model (depth > 3.0 km), shown as purple (i.e. positive lateral temperature gradient). By comparing with the temperature contours presented in Fig 3.3 (A), the temperature field displays as a constant decreased in temperature. However, fluid was observed to flow with slight concave contour. Heat gradient is seen to be positive at those regions, which is reflected as a probable Au dissolution region. RAI was observed to be negative at the lower centre seen in Fig 3.3 (B), suggesting positive heat gradient present in that region.

In summary, M2 simulation provided a benchmark on the conservative thermal field generated in Ellipsis while assuming a metamorphic permeability-depth decay function. The fluid vectors and streamlines show fluid circulation, creating up to two possible elliptical convective cells despite a boundary effect. The presence of these cells suggests that conditions for a localised fluid convection was achieved despite a diffusive flow dominance. The implementation of $RAI_{Au}$ indicated the majority of the model experienced a negative thermal gradient. Positive thermal gradient occupied at the lower half of the cell, concentrating at the centre.

### 3.3.3 M3 and M3 V simulations

The permeability fields in M3 and M3 V simulations are made up of a combination of isotropic and variable permeability fields (Fig 3.1 (M3, M3 V)). The granites present in the simulations were considered as impermeable with an isotropic field of $10^{-18}$ m$^2$. These simulations also contained ‘channel’ geometries relating to the presence of adjacent vertical greenstone bodies. The permeability for these greenstone was set to be isotropic feature at $10^{-14}$ m$^2$ M3 and a variable permeability with values ranging from $10^{-19}$ to $10^{-12}$ m$^2$. $Pe$ values were evaluated to approach 122.0 for M3 indicating advective flow dominance.
whereas, Peclet values for M3V reached 0.0579 indicating diffusive flow dominance. Thus, M3 and M3 V were simulations of fluid movement and RAI in a single greenstone channel or keel in different permeability conditions. The steady-state solution was examined to determine areas for possible fluid convection.

The fluid regime in M3 (Fig 3.4 (A)) was observed to lead to the formation of multiple convection currents seen from the fluid vectors in all areas of the greenstone. The size of the convection cell varies from the width of the greenstone channel (2.75.0 km) to 3.75 km. Fluid flux plotted for M3 (Fig 3.4 (A)) is constrained to $10^{-8}$ to $10^{-10}$ m.s$^{-1}$ showing fluid flow patterns as an outcome from possible metamorphic induced flow. The faster convection current was formed as a result of the presence of the greenstone channel. The fluids at the base of the greenstone channel were heated at higher temperatures ($\sim 100^\circ$ C), generating a higher fluid pressure that decreased laterally at the egress of the channel.

Like in M1, the areas for mineralization were found at the lower half of the convection cell due to a negative lateral thermal gradient. The region for negative lateral thermal gradient at the greenstone cover (left green arrow of 3.4 (B)) was much thinner due to a lower temperature field in its vicinity. RAI’s sensitivity to thermal gradients was reinforced from M2 and M1, showing a similar pattern to M1’s model wide convection cell.

The fluid regime in M3 V (3.5 (A)) was observed for fluids in an upward draft motion, with gravity-driven flow overpowering any possibility for free convection (Oliver et al. [74]). High fluid flux was found at the base of the channel towards the surface, providing a channelling effect described in Cox [18]. At the sides of the channel, fluids were observed to advect towards the surface suggesting driven by gravity-hydraulic flow. Fluid movement was seen to converge towards corners of the model as the corners of the models were set as impermeable. This upward draft implied that conditions for fluid convection have not been reached due to the lack of higher permeability regions. Since the conditions for fluid convection were not met, the fluids do not undergo any form of circulation. Another reason
Fig. 3.4 Simulation outputs for M3. (A) shows fluid flux with temperature contours and dimensionless infinitesimal fluid vector overlay. (B) shows outcome of the application of \( RAI/Au \) with fluid circulations (green arrows) as streamlines. Streamlines in (B) were plotted for a portion of the model for clarity. Colour bars below each subfigure display fluid flux (A) and relative potentials of probable precipitation of Au (negative, red) and probable dissolution of Au (positive, blue).

Fig. 3.5 Simulation outputs for M3 V. (A) shows fluid flux with temperature contours and dimensionless infinitesimal fluid vector overlay. (B) show outcome of the application of \( RAI/Au \) with streamlines. Colour bars below each subfigure display fluid flux (A) and relative potentials of probable precipitation of Au (negative, red) and probable dissolution of Au (positive, blue).
is the feedback from the channelling of fluids from the greenstone channel. Fluids flow from the channel will be met with the impermeable fluid boundaries, consequently pushing the percolating fluids from the cover towards the corner shown in the streamlines (Fig 3.5 (B)).

The application of RAI (3.5 (B)) provides the limited regions of positive (positive RAI) and negative (negative RAI) lateral temperature gradients at the base of the channel. The greenstone cover lies above the channel exhibiting limited regions for thermal gradients, inferring minor changes to the over thermal regime. Within the greenstone channel, negative thermal gradients (Red) was experienced at the base and the left side of the channel. Regions for positive lateral thermal gradients (blue) were observed at the base of the channel. Streamline plots in the channel indicated little deviation of fluids, inferring unfilled conditions for fluid convection. The fluid movement from Fig 3.5 (A) and RAI patterns in Fig 3.5 (B) were observed to flow from the permeability interface before advecting. We infer that the channel is heated by the granites and possibly driven from the abrupt increase in permeability.

In summary, high permeability within the greenstone encourages fluid migration towards the surface, providing the means for fluid circulation within the channel and in the cover (3.4). However, under a variable permeability setting (Fig 3.5), the greenstone channel continues to play as the channelling agent for fluids to percolate to the surface. The RAI output for M3 is more defined than M3 V due to the presence of convective cells. Although the fluid channelling effect was observed in M3 V, the channel was not able to fulfill the conditions for fluid convection.

### 3.3.4 M4 and M4 V simulations

The permeability and geology profiles for both M4 and M4 V simulations present a scenario similar in M3 and M3 V. Instead of simulating fluid flow in a single greenstone keel or channel, this model aims to conduct fluid flow that mimic the effect of multiple greenstone channels and accommodating granitic domes seen in the East Pilbara Craton (Fig 3.1 (M4...
and M4 V)). To maintain the same model dimensions and thermal output from the previous models, the spatial dimensions for the additional greenstone channels were made smaller. Like the previous simulations except for M1, determination for fluid convection cannot depend on the evaluation of the Rayleigh number. M4 had a calculated \( Pe \) value of 125 stating advective flow dominance. M4V however, had \( Pe \) values of 0.38 stating diffusive flow dominance.

Fig. 3.6 Simulation outputs for M4. (A) shows fluid flux with temperature contours and dimensionless infinitesimal fluid vector overlay within the greenstone channels and cover. (B) shows outcome of the application of \( RAI_{Au} \) with fluid streamlines. Localised circulations were observed (green arrow). Colour bars below each subfigure display fluid flux (A) and relative potentials of probable precipitation of Au (negative, red) and probable dissolution of Au (positive, blue).

In M4 simulation, multiple convection currents were observed occurring on the greenstone cover and the channels (Fig 3.6). The presence of these convective cells confirm that the conditions for fluid convection had been met. Peak fluid flux was observed at the base of each greenstone channel and on selected regions in the greenstone cover. The 40° temperature contour at the right side of Fig 3.6 (A) was observed to be slightly lower than on the right side. The lower thermal gradient and the adjacent convection current implied the transition from higher to lower energy states.
When RAI was implemented into M4 (Fig 3.6 (B)), two contrasting regions of lateral thermal gradient located at the channels and within the greenstone cover. RAI indicates alternation of positive and negative thermal gradients across the cover adjacent to the granitic domes. Streamline plots at selected greenstone covers adjacent to the domes confirmed the presence of fluid circulation. However, the fluid movement and RAI patterns in the channels were not defined as well. Each channel experienced a similar amount of positive and negative regions. The streamlines suggest convection (green arrows at channels in Fig 3.6 (B)).

Fig. 3.7 Simulation results for M4 V. (A) shows fluid flux with temperature contours and dimensionless infinitesimal fluid vector overlay within the greenstone channels and cover. (B) shows outcome of the application of $RAI_{Au}$ with fluid streamlines. Colour bars below each subfigure display fluid flux (A) and relative potentials for probable precipitation of Au (negative, red) and probable dissolution of Au (positive, blue).

Under a variable permeability channel setup in M4V (3.7 (A)), the fluid regime was observed to form alternating regions of lower fluid flux and higher (or channelled) fluid flux. The difference in fluid flux between the flux regions was up to two orders of magnitude. The higher fluid flux regions were accompanied with the greenstone channels and peak fluid flux was observed at the base of the channels. The heightened fluid flux readings re-affirmed the channelling effect of fluid from the greenstone channels. The vectors present within the fluid
vectors were seen to converge to a certain point near the surface. These areas of convergence were located near the surface adjacent to a higher flux region.

RAI and streamline were applied to M4 V (Fig 3.7 (B)). The converging behaviour of fluids shown by the vectors in Fig 3.7 (A) was observed to create localised circulation. The presence of these circulations (green arrows) suggest that the fluid regime has met the conditions for fluid convection despite having diffusive flow dominance. The RAI patterns observed in M4 V (Fig 3.7 (B) were similar to M3 V (Fig 3.5 (B)) with any potential Au mineralisation at the base of the channel. Gravity-driven flow is the most prominent within the greenstone channels.

M4 and M4 V simulations introduced additional greenstone channels from M3 and M3 V simulations to approximate a multiple dome and basin setting found in the East Pilbara Craton. The conditions for fluid convection were achieved with the formation of convection currents in M4 and M4 V simulations. The presence of these channels under isotropic and variable permeability created regions of higher fluid fluxes, complementing the fluid focusing mechanism in a more restrictive permeable matrix (e.g. Phillips 1991, Cox et al. 2001). The implementation of RAI suggest a possible asymmetrical behaviour of fluids pertaining to thermal gradient.

3.4 Chapter Summary

Ellipsis3D, coupled with a fluid flow simulator (SHEMAT) followed by the implementation of RAI (Phillips 1991, Zhao 2000), was applied on a variety of simulations of increasing complexity. These simulations mimic static conditions of the generic Precambrian granite-greenstone setting. M1 acted as the benchmark model modified from the Elder (1967) model, observing the presence of a convective cell. Conditions appealing to potential Au mineralisation were found at the lower half of the convective cell. M2 was another benchmark model in a different permeability setting, creating the conditions for a pair of convection
currents near the surface. Distribution of heat from the lower thermal boundary was inferred to be uneven creating alternating regions of positive and negative lateral thermal boundaries.

M3 and M4 simulations experimented with the implementation of greenstone channels of different geometries. Higher fluid flux was seen at the ingress and egress of the channels in an isotropic permeability setting on greenstone channels. Fluid convection was also observed at the greenstone cover. When the permeability of the greenstones shifted to a variable permeability setting, fluid convection was limited while maintaining a higher fluid flux within the channels. The additional channels in M4 V provided the conditions for limited fluid convection through the observation of convection currents.

The experimentation with different permeability fields of increasing complexities continues to reinforce permeability’s influence to the fluid flow regime.
Chapter 4

Crustal Fluid flow in Mesoarchean Granite-Greenstone Terrane: Example of the East Pilbara Craton

4.1 Preamble

In a recent publication, Thébaud and Rey (2013) documented their two-dimensional numerical simulations on the thermal evolution of Mesoarchean greenstones as they sink into a less dense, hot and weak felsic crust. Comparing of this thermal evolution to the thermal evolution recorded in the Paleoarchean to Mesoarchean Warrawoona synform (Eastern Pilbara Craton, Western Australia), the authors proposed that gravity-driven tectonics in a hot and flooded setting had been capable in driving long-lived mineralisation systems away from continental margins, thus providing the fluid pathways needed for promoting Au mineralisation and concentration (Thébaud and Rey 2013).

In the previous chapter, fluid flow simulations were described on generic models of increasing complexities in geology and permeability fields in the previous chapter. A one-way coupling was established using temperature data from Ellipsis into SHEMAT for fluid
flow. In this chapter, the fluid flow workflow designed as part of this study is applied to a series of outputs from the original thermo-mechanical simulation presented in Thébaud and Rey (2013). The results obtained are then evaluated to map out fluid flow patterns and their implications for ore deposit formation in a complex Mesoarchean granite-greenstone context.

4.2 Geological and modelling background

4.2.1 Geological and structural setting

The granite-greenstone terrae in the East Pilbara Craton, Western Australia preserves an ancient geological history largely overprinted in many Neoarchean cratons. Granitic domes largely consist of c. 3,324 to 3,300 Myr old syn- to post- kinematic suites of K-rich granitic suites. These K-rich granitic suites are derived from older c. 3,460 to 3430 Myr, intrusive in Tonalite-Trondjhemite-Granodiorite (TTG) gneisses and greenstones of the Warrawoona Group (van Kranendonk et al. 2007, 2002[111, 112], Hickman and van Kranendonk 2004, Smithies et al. 2003, Hickman 1983). These granitic suites forming the domes are themselves intruded by younger granitoids dated at c. 3,300 to 3,240 Myr old granites. The older TTG gneisses are interpreted to form the basement over which the greenstones were deposited. The emplacement of the greenstone package is associated with two major volcanic cycles: the deposition of Warrawoona Group at ca. 3,490 Myr and the deposition of the Kelly Group at ca. 3,335 Myr (van Kranendonk et al. 2007). The thickness of the greenstone covers exhibit substantial thickness lateral variation from 8 to 12 km for the Warrawoona Group, and 4 to 9 km for the Kelly Group (e.g. van Kranendonk et al. 2007, Hickman 1983).

4.2.2 Ellipsis-SHEMAT workflow

The following simulations were processed in a three-step workflow (Fig 4.1).
Fig. 4.1 The three-step Ellipsis-SHEMAT workflow used for conducting EPC simulations. Step 1 involves the reproduction of the initial thermo-mechanical experiment from Thébaud and Rey (2013) leading to the selection of the appropriate Ellipsis time steps. Data (Geology, Temperature and Strain-rate) from selected time steps are then extracted and translated into a format usable for SHEMAT. Step 2 assigns all known geological and thermal parameters to run the fluid flow simulation. Step 3 goes into the post-processing the output from SHEMAT, generating plots and visualisation maps for fluid flux, RAI, permeability and etc.
The first step utilises a thermo-mechanical code, Ellipsis. This is a Lagrangian integration point finite element code capable of tracking time dependent variables in combination with an Eulerian mesh. This coupled Lagrangian/Eulerian approach allows for accurate tracking of density interfaces during large deformation cycles (Moresi et al. 2002, 2001, [67]). The process utilizes viscoplastic rheologies that mimic standard rheological profiles for the continental lithosphere (e.g. Brace and Kohlsteadt 1980). Realistic geothermal gradients with self-radiogenic heating and partial melting with feedback on viscosity and density were also included in the experiment. Time steps of the thermo-mechanical experiment were reviewed and chosen based on their representation of the sagduction process of the granite-greenstone terrane.

Three data arrays were taken from the selected time steps from the particles files namely; Geology, Temperature and Strain-rate. These data arrays is then translated into the appropriate data structure usable for SHEMAT with the aid of Python and PySHEMAT (Wellmann et al. 2012), a Python plugin for SHEMAT. The geometry, thermal and geological properties and boundary conditions of EPC model were determined in this step. The resultant permeability field was computed and inserted into the SHEMAT input file.

The output files for SHEMAT were then post-processed. The Neumann, Courant and Peclet criterion values were evaluated to determine overall numerical stability. Peclet numbers were then extracted and presented for each model to highlight diffusive or advective flow dominance. Text based output files (.nlo) were post-processed within Python via the PySHEMAT plugin, facilitating the calculation of several important variables such as Permeability and Fluid velocity. The corresponding visualisation files (.vtk) were viewed in Paraview to map fluid vectors and streamlines, determining the occurrence for possible convection cells.
4.2.3 Thermo-mechanical model setup and results

The thermo-mechanical experiment conducted in this study reproduced the original modelling setup as set out by Thébaud and Rey (2013) including the thermo-mechanical properties is presented in Table 4.1. Similar to the original thermo-mechanical simulation the model included a greenstone cover comprising the Warrawonna and Kelly groups. During the thermal incubation of the greenstone packages, no mechanical damage was found in between the greenstone-basement interface. This observation is consistent with field observations of the concordant contact between the Kelly Group and the Warrawoona Group (Van Kranendonk et al. 2004) and the original thermo-mechanical simulation (Thébaud and Rey 2013). It validates the use of similar thermo-mechanical properties to the greenstone packages. The combined 15 km thickness of these groups is also consistent with the average thicknesses of many Archean greenstone covers (e.g. Van Kranendonk et al. 2007). This original geometry was however, slightly altered from the original model. Two small topographic variations of the basement/greenstones interface were introduced (120 km and 240 km sections seen in 4.2 (a) as red circles) in order to reduce the time taken for Rayleigh-Taylor instability to occur. The greenstones were emplaced on a 30 km thick basement with its depth-independent density of 2720 kg.m$^{-3}$. The density of the greenstones remains unchanged from the original study (2840 kg.m$^{-3}$) and it compares well with the results from gravity modeling of the greenstone terrane (Blewett et al. 2004).

Ellipsis provides snapshots of the evolution of the area. Each time-step shown in Fig 4.2 will be used to illustrate the phases the sagduction process.

In Fig 4.2 (a) and (b), the model exhibits the thermal incubation associated with the initiation of gravitational instability. The lower Warrawoona group begins to experience localized thickness variations as a consequence of the granite’s upwelling. Moments later, the Warrawonna group begins to ‘sink’, causing the granites to rise passively as accommodation structures, seen in 4.2 (c) (Van Kranendonk and Collins 1998). The convergence of the
<table>
<thead>
<tr>
<th>Parameters</th>
<th>Value(s)</th>
<th>Unit</th>
</tr>
</thead>
<tbody>
<tr>
<td>(a) Rheological properties</td>
<td></td>
<td></td>
</tr>
<tr>
<td>$g$: Acceleration of gravity field</td>
<td>9.81</td>
<td>m/s$^2$</td>
</tr>
<tr>
<td>$\rho_{atm}$: Air density</td>
<td>2.0</td>
<td>kg/m$^3$</td>
</tr>
<tr>
<td>$\rho_{CFB}$: CFB density</td>
<td>2.0</td>
<td>kg/m$^3$</td>
</tr>
<tr>
<td>$\rho_{cr}$: Crustal density</td>
<td>2.0</td>
<td>kg/m$^3$</td>
</tr>
<tr>
<td>$\rho_{mc}$: Mantle density</td>
<td>2.0</td>
<td>kg/m$^3$</td>
</tr>
<tr>
<td>$C_{CFB}$: CFB cohesion</td>
<td>10</td>
<td>MPa</td>
</tr>
<tr>
<td>$C_{cr}$: Crustal cohesion</td>
<td>10</td>
<td>MPa</td>
</tr>
<tr>
<td>$C_{mc}$: Mantle cohesion</td>
<td>40</td>
<td>MPa</td>
</tr>
<tr>
<td>$\epsilon_{eq}$: Strain weakening factor</td>
<td>0.2</td>
<td></td>
</tr>
<tr>
<td>$\epsilon_{c}$: Strain from which weakening is maximum</td>
<td>0.2</td>
<td></td>
</tr>
<tr>
<td>$\epsilon_{c}$: Strain weakening sensitivity to accumulated strain</td>
<td>0.5</td>
<td></td>
</tr>
<tr>
<td>$\sigma_{gc}$: Greenstone maximum yield stress</td>
<td>100</td>
<td>MPa</td>
</tr>
<tr>
<td>$\sigma_{gcr}$: Granite maximum yield stress</td>
<td>250</td>
<td>MPa</td>
</tr>
<tr>
<td>$\sigma_{mc}$: Mantle maximum yield stress</td>
<td>400</td>
<td>MPa</td>
</tr>
<tr>
<td>$\phi_{gc}$: Greenstone internal angle of friction</td>
<td>5</td>
<td></td>
</tr>
<tr>
<td>$\phi_{gcr}$: Granite internal angle of friction</td>
<td>15</td>
<td></td>
</tr>
<tr>
<td>$\phi_{mc}$: Mantle internal angle of friction</td>
<td>25</td>
<td></td>
</tr>
<tr>
<td>$\eta_{atm}$: Air viscosity</td>
<td>5 x 10$^{26}$</td>
<td>Pa.s</td>
</tr>
<tr>
<td>$A_{gc}$: Greenstone pre-exponent constant</td>
<td>5 x 10$^{-5}$</td>
<td>MPa$^{-n}$s$^{-1}$</td>
</tr>
<tr>
<td>$A_{gcr}$: Granite pre-exponent constant</td>
<td>5 x 10$^{-6}$</td>
<td>MPa$^{-n}$s$^{-1}$</td>
</tr>
<tr>
<td>$A_{mc}$: Mantle pre-exponent constant</td>
<td>7 x 10$^{4}$</td>
<td>MPa$^{-n}$s$^{-1}$</td>
</tr>
<tr>
<td>$n_{gc}$: Greenstone stress exponent</td>
<td>3</td>
<td></td>
</tr>
<tr>
<td>$n_{gcr}$: Granite stress exponent</td>
<td>3</td>
<td></td>
</tr>
<tr>
<td>$n_{mc}$: Mantle stress exponent</td>
<td>3</td>
<td></td>
</tr>
<tr>
<td>$Q_{gc}$: Greenstone activation enthalpy</td>
<td>1.9 x 10$^{5}$</td>
<td>J/mol$^{-1}$</td>
</tr>
<tr>
<td>$Q_{gcr}$: Granite activation enthalpy</td>
<td>1.9 x 10$^{5}$</td>
<td>J/mol$^{-1}$</td>
</tr>
<tr>
<td>$Q_{mc}$: Mantle activation enthalpy</td>
<td>5.2 x 10$^{5}$</td>
<td>J/mol$^{-1}$</td>
</tr>
<tr>
<td>$R$: Gas constant</td>
<td>8.3145</td>
<td>J/mol$^{-1}$K$^{-1}$</td>
</tr>
<tr>
<td>(b) Thermal properties</td>
<td></td>
<td></td>
</tr>
<tr>
<td>$\alpha_{mc}$: Mantle coefficient of thermal expansion</td>
<td>2.8 x 10$^{-3}$</td>
<td>K$^{-1}$</td>
</tr>
<tr>
<td>$\kappa$: Thermal diffusivity</td>
<td>0.9 x 10$^{-6}$</td>
<td>m$^2$s$^{-1}$</td>
</tr>
<tr>
<td>$C_{p}$: Heat Capacity</td>
<td>1000</td>
<td>J kg$^{-1}$K$^{-1}$</td>
</tr>
<tr>
<td>$H_{CFB}$: CFBs heat production</td>
<td>1.335 x 10$^{-7}$</td>
<td>Wm$^{-3}$</td>
</tr>
<tr>
<td>$H_{cr}$: Crustal heat production</td>
<td>1.335 x 10$^{-6}$</td>
<td>Wm$^{-3}$</td>
</tr>
<tr>
<td>$H_{mc}$: Mantle heat production</td>
<td>0</td>
<td>Wm$^{-3}$</td>
</tr>
<tr>
<td>$q_{mc}$: Basal mantle heat flux</td>
<td>0.025</td>
<td>Wm$^{-2}$</td>
</tr>
<tr>
<td>(c) partial melting parameters</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Latent heat</td>
<td>250</td>
<td>LJ</td>
</tr>
<tr>
<td>Greenstone:</td>
<td></td>
<td></td>
</tr>
<tr>
<td>- Solidus (P)</td>
<td>993 – 1.2 x 10$^{-7}$P + 1.2 x 10$^{-16}$P</td>
<td>°C</td>
</tr>
<tr>
<td>- Liquidus (P)</td>
<td>1493 – 1.2 x 10$^{-7}$P + 1.2 x 10$^{-16}$P</td>
<td>°C</td>
</tr>
<tr>
<td>Granite:</td>
<td></td>
<td></td>
</tr>
<tr>
<td>- Solidus (P)</td>
<td>983 – 9.37 x 10$^{-8}$P + 6.32 x 10$^{-17}$P</td>
<td>°C</td>
</tr>
<tr>
<td>- Liquidus (P)</td>
<td>1393 – 9.37 x 10$^{-8}$P + 1.2 x 10$^{-17}$P</td>
<td>°C</td>
</tr>
</tbody>
</table>

Table 4.1 Thermo-mechanical simulation properties taken from [103].
Chapter 4  Poh’s M.Sc Thesis

Basal Heat flux = 0.025 W.m$^{-2}$

$T_0 + 3.02$ 3Myr (a)

(b) $T_0 + 3.77$ 3Myr  

(c) $T_0 + 3.77$ 3Myr

(d) $T_0 + 3.99$ 5Myr

(e) $T_0 + 4.14$ Myr

(f) $T_0 + 4.90$ Myr

Fig. 4.2 Initial numerical settings and time-steps of the reproduced thermo-mechanical experiment. Blue shading shows post yielding plastic strain. In each figure, dotted white line in each figure shows the depth of 10 km. Arrows pointing at passive vertical markers (red dots) in the granite documents the deformation pattern. Red circles in (a) refer to small variations of greenstones near the contact points to decrease time taken to achieve Rayleigh-Taylor instability.

Numerical simulation initial setting

<table>
<thead>
<tr>
<th>Material</th>
<th>Density (kg.m$^{-3}$)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Greenstones</td>
<td>2840</td>
</tr>
<tr>
<td>Granite</td>
<td>2720</td>
</tr>
<tr>
<td>Air</td>
<td></td>
</tr>
<tr>
<td>Kelly Group</td>
<td></td>
</tr>
<tr>
<td>Warrawonna Group</td>
<td></td>
</tr>
<tr>
<td>Granite and partial melting</td>
<td></td>
</tr>
<tr>
<td>Mantle</td>
<td></td>
</tr>
</tbody>
</table>

Basal Heat flux = 0.025 W.m$^2$

100 km

15 km

30 km

57
tracking points (red dots in Fig 4.2) were observed to document the crustal overturn effect. Compared to the original thermo-mechanical experiment, the onset of gravitational instability occurred much faster as a consequence of the modified model’s initial geometry. Nevertheless the results showed a similar sagduction process comparable with those of the original model (Thébaud and Rey 2013).

Fig. 4.3 Temperature profile at 10km depth, from \( t_0 + 3.773 \) to \( t_0 + 4.439 \) myr, building up a thermal anomaly. The upwelling of the granitic domes creates a significant horizontal temperature difference.

The thermal evolution calculated in the reproduction of the Ellipsis simulation displayed a similar thermal history compared to the original experiment (Fig 4.3). From the onset of sagduction at \( t_0 + 3.773 \) Myr (blue line) to \( t_0 + 4.439 \) Myr (green line), advection of cooler greenstone rocks experienced a downward flow in downwelling regions where the temperature at 10 km decreases from 350° to 150° C (Fig 4.3). In contrast, the temperatures in the rising domes at 10 km increased from \( \sim 425° \) to 742° C (Fig 4.3). At about 4.4 myr, partial convective overturn led to the build up of a long-wavelength (lateral distance of 100 km) lateral thermal anomalies 500° C through fast advective cooling and heating of downwelling
and upwelling regions respectively. The maximum horizontal temperature gradient reaches 10.745° C/km, two times smaller than the original simulation of 26° C/km. The reproduced model’s modified greenstone/basement topography from the original model is likely to create a different result despite using identical thermo-mechanical conditions. (shown as red circles in Fig 1.2 (A)). On the whole, the experiment yielded an outcome comparable with those of the original model (Thébaud and Rey 2013), from the generation of thermal peaks from the upwelling of hotter granites and thermal troughs from the downwelling cooler greenstones.

4.2.4 SHEMAT model setup

For fluid flow simulation, data from each Ellipsis time-step, such as geology, temperature and strain-rate ($\dot{\varepsilon}$), were transferred to SHEMAT for fluid flow simulation. All EPC simulations will have the same model dimensions; a horizontal extent of 225 km and a vertical extent of 46.5 km. This gives a total cell count of 167,400 cells.

The thermal boundary conditions for EPC 1 to 5 simulations were constant with the initial temperature fields imported from Ellipsis. The horizontal thermal boundaries are kept at constant temperature, which gives the top interface a constant temperature of $\sim 21.8^\circ$ C, reflecting typical atmospheric conditions. The lower thermal boundary has a constant temperature up to $\sim 800^\circ$C at 40km depth, which assumes constant heating from the mantle. This thermal regime provides a stable geothermal gradient of 19.46° C/km, comparable for a tectonically stable continental crust (e.g. Ranalli [79]). The geothermal gradient peaks at 35 km and 175 km marks from 4.3 up to 75.0° C/km from upwelling of the granites. If the mantle is present within the SHEMAT simulation, their temperature will be held as constant. Heat flux is kept at 0.025 W.m$^{-2}$ to be consistent with the thermo-mechanical model. Finally, all boundaries of the model were set as impermeable, creating conditions for a closed system with one heating element.
Initial fluid flow was driven by a reference hydraulic head according to the vertical extent of the model (Table 4.2, Initial hydraulic head). The porosity in all simulations was set to 1% regardless of the rock type or permeability. This simplification was done under the assumptions taken in the following simulations, as the effect on the flow regime and porosity is negligible (Kuhn et al. 2006), representing the lowest value most conservative value required in SHEMAT (Clauser 2003). Rocks at depth (7 km from the surface) will experience lithostatic pressure up to 200 MPa (Rutqvist 2015), capable of overcoming the resistant effect of pore-fluid pressure under any deformation.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
<th>Unit</th>
</tr>
</thead>
<tbody>
<tr>
<td>Initial hydraulic head</td>
<td>46 500</td>
<td>m</td>
</tr>
<tr>
<td>$k_{gr}$: Granite permeability</td>
<td>$10^{-20}$</td>
<td>$m^2$</td>
</tr>
<tr>
<td>$k_m$: Mantle permeability</td>
<td>$10^{-20}$</td>
<td>$m^2$</td>
</tr>
<tr>
<td>$k_{gs}$: Greenstone permeability</td>
<td>$10^{-12} - 10^{-19}$</td>
<td>$m^2$</td>
</tr>
<tr>
<td>$c_{gr}$: Granite thermal conductivity</td>
<td>2.559</td>
<td>$W.m^{-1}.K^{-1}$</td>
</tr>
<tr>
<td>$c_m$: Mantle thermal conductivity</td>
<td>2.448</td>
<td>$W.m^{-1}.K^{-1}$</td>
</tr>
<tr>
<td>$c_{gs}$: Greenstone thermal conductivity</td>
<td>2.979</td>
<td>$W.m^{-1}.K^{-1}$</td>
</tr>
<tr>
<td>$\kappa_{gr}$: Granite thermal capacity</td>
<td>1.0</td>
<td>$J.kg^{-1}.K^{-1}$</td>
</tr>
<tr>
<td>$\kappa_m$: Mantle thermal capacity</td>
<td>1.0</td>
<td>$J.kg^{-1}.K^{-1}$</td>
</tr>
<tr>
<td>$\kappa_{gs}$: Greenstone thermal capacity</td>
<td>1.0</td>
<td>$J.kg^{-1}.K^{-1}$</td>
</tr>
<tr>
<td>$\phi$: Porosity</td>
<td>0.01</td>
<td>-</td>
</tr>
</tbody>
</table>

Table 4.2 Model properties used in SHEMAT

Using strain-rate in estimating dynamic permeability

Rock permeability is described as a measure of the relative ease of fluid under unequal pressure (Chapter 2). The range of permeability in rocks spreads over 16 orders of magnitude ranging from intact granitic rocks at $k = 10^{-20}$ m$^2$ to fractured basaltic rocks at $k > 10^{-11}$ m$^2$ (e.g. Ranjram et al. 2015, Rutqvist 2015, Rutqvist and Stephansson 2003). The level of uncertainty assigned to permeability was very high due to its anisotropy both through time and lateral and vertical distances (e.g. McCuaig and Hronsky 2014, Cathles and Adams 2005, Cox et al. 2001). To overcome this challenge, this chapter aims to calculate a first
approximation of 'dynamic permeability' through the use of strain-rate, $\dot{\varepsilon}$ in a pre-defined background permeability.

The concept of 'Dynamic permeability' (Cathles and Adams 2005) describes the complexity of changes in permeability through time. Permeability can be altered through a variety of processes such as chemical alteration (e.g. Rutqvist and Stephansson 2003, Phillips 1991, ), hydraulic forces (e.g. Sibson 2004), crustal seismological activity (e.g. Micklethwaite et al. 2015, Sibson 2001), a coupled process (e.g. Hobbs 2000) or an integration of all possible processes. Simulating dynamic permeability requires a coupling of at least two or more processes to approach a realistic system. The numerical codes used in this dissertation do not have the capacity of evaluating dynamic permeability. Ellipsis (introduced later in this chapter) simulates a dynamic thermo-mechanical evolution over a long time periods. SHEMAT however, is capable of simulating fluid flow in a static model.

Due to the limitations in the numerical tools, our approach to evaluating 'dynamic permeability' involves a 'one-way' coupling: only combining the results from one simulation as a proxy for the expected spatial distribution of high permeability regions. This mapping is motivated with the expectation of high strain zones as 'snapshots' of crustal seismological activity over a longer time range. This approach may not be ideal but it is suitable for modeling a first approximation for the sagduction process. Pursing a method to simulate a fully coupled dynamic permeability is out of the scope of the dissertation but it remains relevant issue for further research.

The permeability field was evaluated from the permeability-depth decay function (Ingebritsen and Manning 1999), where permeability, $k \ (m^2)$, depth $z \ (km)$ and strain-rate, $\dot{\varepsilon}$ are adjusted by a constant, $c$, expressed in Eqn 4.1. The premise is to integrate the effects of deformation and fluid flow. But SHEMAT and Ellipsis are unable to perform this automatically. Since the focus of this work is to establish the conditions of fluid flow in the greenstone package during dome and basin formation, the dynamic permeability was solely applied to
the greenstones and the granites were assumed to be impermeable and given an isotropic
permeability value of $k = 10^{-20}$ m$^2$.

$$\log k = (-14 - 3.2 \log z) + (\log \dot{\varepsilon} - c)$$ (4.1)

Relating strain-rate to form dynamic permeability is derived from the propagation and
healing of fractures through seismicity events with hydrothermal fluid flow. The creation of
faults and shear zones is essential for transient permeability enhancements as it allows the
migration of large volumes of fluids through narrow spaces (e.g. Cox 2001). This migration
of fluids is instrumental in the healing of fault systems leading to in permeability decay,
as observed in hydrothermal deformation experiments (e.g. Kay et al. 2006), post seismic
monitoring of groundwater geochemistry (e.g. Rojstaczer et al. 1995) and the variations in
seismic wave speeds in newly established fault systems (e.g. Tadokoro and Ando 2002). The
time taken to restore a fractured domain was up to 10 years (e.g. Rolandone et al. 2004,
Kitagawa et al. 2007). Recent fluid modeling on a fault step over system estimated that
damage zones could be healed in less than 30 years (Micklethwaite et al. 2015). This affirms
the time-sensitivity of any permeability enhancement and decay (e.g. Micklethwaite et al.
2015, Cathles and Adams 2005). The implementation of strain-rate provides the avenue in
seeing fluid flow from the enhancement of permeability through short-lived shear zones.

The relationship between strain-rate and permeability enhancement remains unclear
despite five decades of experimental work. Previous studies were conducted to quantify
the relationship of stress and resultant rock permeability on granite (Brace et al. 1968),
aquifer (Yin and Wang 2006[121]) and samples from an active fault zone (Morrow et al.
2015). These studies concluded that permeability decay is an outcome of increasing confining
pressure. However, as strain-rate was not explored in these studies, its relationship remains
unclear. Given the understanding that damage zones described in Micklethwaite et al. 2015
are short-lived, the change of permeability is assumed to have a linear relationship with strain-rate, making this a conservative first approximation. The proposed relationship will preserve short-lived zones at depth before healing process from hydrothermal fluids can begin.

Establishing a simple linear relationship with strain-rate and background permeability will be challenging without any guidelines from previous studies. Subsequent simulations were undertaken to test varying degrees of effectiveness of strain-rate to permeability on the East Pilbara Craton (later described in this chapter), seen in Fig 4.4. All models in Fig 4.4 are taken at steady-state conditions: constant temperatures at the upper (21.7°C), lower boundaries (∼750°C), and impermeable fluid boundaries in the model.

With no alterations to strain-rate (c = 0), the shear zones seen in Fig 4.4 (A1) have the permeability of $10^{-13}$ m$^2$ at 25 km depth. Such drastic changes in permeability induces a difference of one order of magnitude in fluid velocity in low and higher permeability regions. Enhanced permeability regions would become susceptible for fluid convection to occur and decreasing overall geotherm (temperature contour of 100°C at the base of greenstone in Fig 4.4 (A2)). Sandstone-like permeability ($k \sim 10^{-12}$ m$^2$) at depths of 25 km would be considered as unrealistic due to the high lithostatic pressure (∼200 MPa at 7km depth), capable of repairing any crack-enhanced permeability (Rutqvist 2015).

Our first alteration to strain-rate is to reduce its effect by two orders of magnitude (c = 2). This alteration provided the greenstone channel network with additional detail. The channel’s average width is 7.0 km with a resultant permeability of $10^{-14}$ m$^2$, as shown in Fig 4.4 (B1). The geometries of the regions of lower permeability ($10^{-16}$ m$^2$) were observed, highlighting the anisotropy in the distribution of strain. Fluid circulation and increases in fluid velocity were observed in the velocity field, shown in Fig 4.4 (B2). These increases in fluid velocity were found in parts of the channel confirming the presence of fluid focusing, similar to our finding in M3 and M4 from Chapter 3. However, a build up of higher fluid
Fig. 4.4 Sensitivity of C with (A1, B1 and C1) as the resultant permeability. (A2, B2 and C2) show fluid movement through streamlines.
velocity (up to $10^{-6}$ m.s$^{-1}$) was observed to be temperature bounded ($100^\circ$C temperature contour) located in the lower permeability regions. This fluid behaviour suggests fluid overpressure (Sibson 2004) at depth, capable of transporting fluids to the surface. In addition, the resultant thermal field improved significantly with the $100^\circ$C at 12.5 km, compared to the $100^\circ$C in Fig 4.4 (A2) at $\sim$ 25 km. At $c = 3$, the greenstone channels have a permeability of $10^{-15}$ m$^2$. This created conditions that restricted fluids from undergoing convection (Fig 4.4 (C1)). The temperature field which moved towards the surface ($100^\circ$C $\sim$ 5 km) improved significantly compared to the previous figures. The fluid flow resulted in an upward through flow while following the contours of the channels. The fluids now appear to converge to certain locations, creating the possibility of potential fluid pathways.

The local sensitivity study concludes that the decrease in the influence of strain-rate (by raising the value of $c$) would lead to the improvement of resultant geothermal field at the cost of overall fluid activity. At the same time, the increase of strain-rate (by decreasing the value of $c$) would improve fluid activity at the cost of generating unrealistic permeability fields at depth and a lower geothermal gradient. Therefore, by assigning a conservative $c = 2.5$ into Eqn 4.1, it provided a reasonable trade off between fluid activity and resultant temperature. However, this warrants a proper sensitivity analysis and in the simulations produced the calculated permeability fields as the fluid flux values are considered as unrealistic and therefore only interpreted in relative terms. In the results section below, the data description therefore focuses on the pattern of fluid flow rather than on both the absolute characterisation of the permeability and fluid flux values.

### 4.3 Fluid Modeling results

EPC 1 to EPC 6 simulations were assessed using their respective resultant permeability fields and their fluid flow regimes. Each simulation provides in a snapshot a time-step through the tectonic evolution of this generic greenstone-granite terrane.
4.3.1 EPC 1 simulation

EPC 1 represents a benchmark model showing fluid flow associated with the incubation period of the deposited greenstone succession over the radiogenic basement at $T_0 + 3.023$ Myr. At that stage of the thermo-mechanical modelling, the greenstone has experienced limited stress and the EPC 1 model fluid flow at a step prior to the main sagduction process. Anomalous strain appears to have locally affected the greenstone succession, forming a vertical corridor at the left side of the model, seen in Fig 4.2 (A).

The calculated permeability field obtained in this model is similar to that modelled through the benchmark model M2 in Chapter 3 (Fig 4.2 (A)). Although strain-rate was observed at the surface, the value of strain-rate was overwritten by the permeability-depth equation. Instead, there was an increase in permeability at the depth of 15km at $k \sim 16.0 \text{ m}^2$ as a result of localised strain during thermal incubation, seen as yellow circles in Fig 4.6 (A).

The $Pe$ value was estimated to reach 1.2, indicating diffusive flow dominance. Fluid flow in EPC 1 could be described as an upwelling flow as a consequence to gravity-hydraulic flow. Fluid flow velocity in strain-enhanced permeability near the granites (yellow circles in 4.5 (A)) was observed to increase by 4 orders of magnitude in 4.5 (B). Fluid flux was observed to remain relatively constant at around $10^{-8} \text{ m.s}^{-1}$ from the depth of 4 km to the bottom of the greenstone, citing similar fluid behaviour in M2 from Chapter 3. Increases of fluid flux were also observed at certain sections of the model 4km depth by an order of magnitude, which indicate regions for fluid convection. Streamline plots in Fig 4.5 (B1) indicate the presence of localised circulations (black arrows).

The upward unidirectional vectors in Fig 4.5 (A) indicate fluid flow driven by gravity-hydraulic flow. These unidirectional vectors suggest that gravity induced flow may overpower any potential localised fluid circulations (Oliver et al. [74]). However, as soon as fluid movement change direction (seen in the vectors in the red box of Fig 4.5 (A)), I can infer additional fluid movement with localised circulations from diffusive flow. A magnified image
of the red box with the corresponding streamlines confirms the presence of such circulations (Fig 4.5 (B1)). The sudden decrease in fluid flux is observed to be thermally driven (\(\sim 100^\circ C\) temperature contour). This suggests that the conditions for fluid convection were met. Therefore, given the current thermal regime, I would expect to see more localised circulations occurring at the surface of the greenstone.

The slight increase in permeability at depth (shown as yellow circles in Fig 4.5 (A)) was similar to the introduction of channels in M3 V and M4 V in Chapter 3. In M3 V and M4 V (Chapter 3), we would expect a sudden increase in fluid flux before decreasing drastically. However, the resultant thermal regime for EPC 1 was observed to be much higher (400\(^\circ\) C at 15 km) than in M3 V and M4 V. The heightened thermal regime provided the means for the fluids to flow towards the surface.

### 4.3.2 EPC 2 simulation

The stage simulated in EPC 2 documents fluid flow prior to the greenstone sagduction at \(T_0 + 3.773 \text{ Myr}\). At that stage the thermal incubation enhanced the partial melting of the lower crust, reducing its viscosity which in turn initiated gravitational instability. Blue shading depicted in Fig 4.6 (b) indicated widespread and anisotropic distribution of the strain-rate at a stage leading to the sagduction of the greenstone into the partially molten basement. The presence of such a distribution suggests domains associated with contrasted permeability. These domains are labelled (1) to (5) in Fig 4.6 (A)). Domains (1), (2), (3) and (5) are associated with low permeability values, implying an unequal distribution of strain. A horizontal yet curved feature of lower permeability with an averaged thickness of 6km was seen in domain (3). Region (4) which is associated with intense strain-rate up to \(10^{-12} \text{ m}^2\) suggests total rock failure. A horizontal followed with a concave lower permeability seal was seen in domain (5).
Fig. 4.5 Permeability and fluid flow results for EPC 1 on $T_0 + 3.023$ Myr. (A) represents the resultant permeability field and the fluid flow arrows. The arrows represent the dimensionless infinitesimal values of fluid movement in the particular time step. Yellow circles highlight areas of strain-enhanced permeability of greenstone near the granite. (B) represents the function for the magnitude of log fluid flux (m.s$^{-1}$). Red boxes in (A) and (B) highlight potential fluid convection to occur in EPC 1, seen in (B1) as the streamline. Localised fluid circulations from (B1) indicated by the green arrows.
The $Pe$ value for EPC 2 was estimated to reach 31600, citing advective flow dominance. The fluid flow regime seen in Fig 4.6 (A) and (B) can be summarized as flowing from the left to the right side of the model, generating convection currents if conditions were fulfilled. The difference in magnitude flowing in regions of higher permeability regions and lower permeability regions is between 1 to 4 orders of magnitude. In permeability (4), fluid circulation occurred near the interface between the greenstone and granite seen in Fig 4.6 (B).

The occurrence of contrasting permeability domains in EPC 2 describes the heterogeneous distribution of strain-rate to the greenstone. Low permeability domains (1), (2), (3) and (5) can be interpreted as low permeability seals applying a structural control leading to fluid overpressure regions (Sibson 2004). The increase in fluid pressure will be capable of inducing hydraulic deformation sequences that is sought after in mineral systems.

Fig. 4.6 Permeability and fluid flow results for EPC 2 on $T_0 + 3.773$ Myr. Resultant permeability field and arrows are dimensionless infinitesimal values of fluid movement (A). (1) to (5) refer to features of strain-enhanced permeability discussed in the text. Fluid flux ($m.s^{-1}$) with streamlines in each numbered permeability feature (B). Localised fluid circulations are identified by black arrows.
4.3.3 EPC 3 simulation

EPC 3 simulation occurs shortly after EPC 2 ($T_0 + 3.773$ Myr), when gravitational instability acted on the greenstone leading to the formation of a greenstone keel or basin. The resultant permeability field displayed a network of strain-enhanced permeability channels with an average width of 3.0 km and several blocks of lower permeability (Fig 4.7 (A)). The strain induced dynamic permeability variation on these channels appear to be capable of increasing $Ra$ for convection currents to occur. The channel network is described as a series of concave and convex features with at least three triple junctions, outlining the limbs of the permeability interface (yellow dashed lines and dots in Fig 4.7 (A)). In the thermo-mechanical simulation, these channels are associated with high strain-rate values ($10^{-12}$ to $10^{-14}$ m$^2$). They are therefore mapping structural conduits that developed in the course of the deformation processes. The fluids were observed to flow along the permeability channels (Fig 4.7(A)) preferably.

Fluid flow was observed to flow from regions of lower permeability to regions of higher permeability (Fig 4.7 (A)). Advective flow dominance was achieved with an estimated $Pe$ value of 1540. Downwelling of fluids were also observed especially in the concave feature (above dotted yellow line at 100 and 200 km horizontal) only to flow along the permeability channels and locally establish convective flow. At the base of the keel, the $100^\circ$ C temperature contour passes through regions of lower permeability at 15 km depth. Streamline plots in Fig 4.7 (B) indicate the presence of several convection currents (black arrows) occurring throughout the greenstone layer. The fluid flux variation in the model displays fluid flowing from regions of lower permeability towards the permeability channels. The peak fluid flux located at 15 km depth was observed to decrease by an order of magnitude, indicating favourable fluid flow within the permeability channel.

A permeability network was established in EPC 3 simulation. It acted as fluid pathways to channel fluids to other areas of the keel. We observed a recurring feature in that the
unidirectional flow was observed at the base of the keel and contained by peak fluid flux (15 km depth). This suggests that the conditions for fluid convection were not met and gravity induced flow was its primary driver. As fluids traverse through the thermal-flux boundary, conditions for fluid convection were met.

Fig. 4.7 Permeability and fluid flow results for EPC 3 on $T_0 + 3.773$ Myr. (A) represents the resultant permeability field and arrows are dimensionless infinitesimal values for fluid movement. Fluid flux plot with streamlines at the different areas of the model (B). Black arrows identify localised fluid circulations. Yellow dotted line in (A) trace the generic shape of the permeability channel network, yellow dots indicate possible triple juncture points for the channels.

### 4.3.4 EPC 4 and EPC 5 simulations

EPC 4 and EPC 5 simulations follow up as advanced greenstone keel development took place. The permeability channels from EPC 3 simulation appear to merge and lead to form two triangular regions of high permeability and a couple of triple junction (Fig 4.8 (A) and Fig 4.9 (A)). Strain-induced permeability in EPC 4 (4.8 (A)) was observed to form a rhombus-like feature of lower permeability at the keel. In EPC 5 (4.9 (A)), this same region starts to ‘break up’ to create an internal network for strain-enhanced channels with the increase to five
inferred vertical triple and quadruple junctions (yellow circles in Fig 4.8 (A) and Fig 4.9 (A)).
The channels appear larger than in the EPC 3 simulation, suggesting a more homogeneous
strain-rate distribution in the greenstone keel as contraction occurs between the two adjacent
rising domes.

Advective flow dominance was achieved with a $Pe$ value of 6480 and 827 for EPC 4 and
EPC 5 simulations respectively. The fluid flow regime was observed to undergo circulation
near the surface in EPC 4 and 5 (Fig 4.8 (A) and Fig 4.9 (A)). This is confirmed by the
streamline plot (Fig 4.8 (B) and Fig 4.9 (B)). These occurrences for fluid circulation were also
observed in close proximity with the thermal-flux boundary interface (bounded by $\sim 100^\circ$ C
temperature contour). High fluid fluxes were observed below the thermal-flux boundary and
within the permeability channels ($> 12.5$ km).

However, from the resultant thermal regime and Fluid flow in EPC 4 and 5 simulations
achieved fluid convection, we infer that the intensity of fluid convection is decreasing as
seen in the size and number of local circulations. The conditions within the channels in
both simulations were suitable for fluid advection, only to be destabilised after breaching the
thermal-flux boundary at $\sim 100^\circ$ temperature contour. Although the channel network from
EPC 3 merged to form two triangular high permeability features in EPC 4 and 5, strain-rate
was seen to become more homogeneous suggesting an onset of tectonic stability. In EPC 5
simulation, the rhombus-like lower permeability was observed to form triple and quadruple
junctions that further suggests a substantial increase in fluid-rock interaction.

4.3.5 EPC 6 simulation

EPC 6 simulation is the final image for the sagduction process at $T_0 + 4.439$ Myr. The
resultant widespread strain-rate permeability field appear to be homogenised over the whole
modelled area. This permeability marks the transition from an heterogeneous distribution of
strain in the model (EPC 3 to EPC 4 simulations) to a more homogeneous strain distribution in
Fig. 4.8 Permeability and fluid flow results for EPC 4 on $T_0 + 3.995$ Myr. (A) represents the resultant permeability field with fluid flow vectors. Yellow lines and yellow circles indicate inferred geometry of strain-enhanced greenstone channels and possible vertical triple or quadruple junctions. (B) show the fluid flux with streamlines at different areas of the model.

Fig. 4.9 Permeability and fluid flow results for EPC 5 on $T_0 + 4.140$ Myr. (A) represents the resultant permeability field with fluid flow vectors. Yellow lines and yellow circles indicate inferred geometry of strain-enhanced greenstone channels and possible vertical triple or quadruple junctions. (B) show the fluid flux with streamlines at different areas of the model.
Fig. 4.10 Permeability and fluid flow results for EPC 6 on $T_0 + 4.439$ Myr. (A) represents the resultant permeability field and arrows are dimensionless infinitesimal values for fluid movement. (B) shows the fluid flux with streamlines at different areas of the model. Black arrows in (B) identifies localized fluid circulation.

EPC 5 and EPC 6 simulations. However, EPC 6 simulation presents two features characterised in the simulation as circular areas of lower permeability and a horizontal beam inferred as a low permeability seal along the $300^\circ$ C contour at each greenstone keel.

The fluid flow regime is dominated by upward through flow with limited development of convection currents despite achieving advective flow dominance with a $Pe$ value reaching 5310. The greenstone keel in the centre has two type of flows. Gravity-induced advective flow was observed occurring from the lower part of the keel with a range of fluid flux from $10^{-10}$ to $10^{-7.5}$ m.s$^{-1}$ whereas limited circulations were observed (black arrows) near the surface. The occurrence of these circulations occur over a fluid flux boundary as fluids transits from gravity induced flow to convective flow with a sudden decrease in fluid velocity of 2 orders of magnitude. These occurrences are not the same for the greenstone keel located at the right side of the model. Gravity-induced advective flow is dominant within that keel with no observable localised circulations within an overall homogeneous permeability field.
Fluid activity in EPC 6 simulation in summary is inferred as minimal, potentially signalling the start of the thermal deflation process.

4.4 Discussion

4.4.1 Fluid flow pattern associated with Mesoarchean gravity driven deformation

Fluid activity in EPC 1 and EPC 2 is associated with minimal fluid activity. The permeability setting in EPC 1 allows for possible localised convection cells near the surface of the greenstone sequence. The majority of the fluid was seen as upward unidirectional advection as a response to be solely driven by hydraulic heading. As thermal incubation progresses seen in EPC 2, the high strain domains start to localise and partition within the greenstone cover. This leads to the formation of high strain-induced permeability domains and low permeability domains or seals. The distribution of these high permeability zones and seals control the fluid’s self-organisation behaviour that is observed in the development of convection cells occurring in the entire greenstone pile.

EPC 3 simulation is associated with the initiation of the sagduction process. It induces strain partitioning along heterogeneous corridors or channels. These channels provide pathways and focal points to encourage funnelling of fluids which is instrumental for fluids to undergo convection. However, the presented channels were found to be channelling fluid flow above a thermal-flux boundary (bounded under 100°C temperature contour). Below this thermal-flux boundary, the fluids experience unidirectional upward advective flow and is accompanied with high fluid fluxes.

EPC 4 and 5 simulations show the evolution of fluid flow patterns as the distribution of strain transitions towards a more homogeneous distribution over the modelled area. Fluid flow is characterised into high and low fluid flux regions, bounded by the recurring thermal-
flux boundary. In the high fluid flux region, upward unidirectional advective fluid flow was observed, indicating that flow was gravity-driven. At the low fluid flux region, localised circulations were observed at the thermal-flux boundary as the development of convective cells. Fluid convection was observed to be declining as the sagduction process matures.

In EPC 6 simulation, the deformation of the greenstone keel has fully matured, resulting in a fairly homogeneous distribution of strain-rate in the modelled area. The calculated dynamic permeability determined a couple of domains of lower permeability, potentially acting as a horizontal seal or a source for metamorphic fluids. Fluid motion below 10 km is governed by a higher fluid flux as gravity-induced flow became more dominant. As fluid passes through the thermal-flux boundary, the conditions for fluid circulation were met. These convective cells occur near the surface. Although the deformation of the greenstone keel has been completed, it was surprising that the level of fluid circulation occurring in EPC 6 simulation is higher than in EPC 5 simulation. It is postulated that fluid activity will continue into the thermal relaxation phase to remain active as long as the conditions for fluid convection are met.

4.4.2 Role of dynamic permeability in establishing an efficient plumbing system

The simulations presented in the this chapter evaluate rock permeability in each time-step of the granite-greenstone permeability on two factors: a permeability decay function (Ingebritsen and Manning 1999) and a linear alteration of strain-rate. The intrinsic permeability of the greenstone is established to account the decay of permeability with an increasing geotherm (Cathles and Smith 1983). The function was chosen as the granite-greenstone terrane can be related to an active geothermal area undergoing metamorphism. As mentioned in Section 4.2.4, the linear relationship between alteration and strain-rate was established to ensure
numerical stability. It was a conservative approach between overall fluid movement and resultant thermal gradient.

The general correlation function in establishing dynamic permeability with strain-rate is non-existent despite having several power laws to evaluate stress-induced permeability. The linear function through the addition of $c$ remains a gross simplification but nevertheless provides a conservative first order approximation. So far, the implementation of Eqn 4.1 allowed the generation of strain-induced channels seen in EPC 3 to 6 simulations. These same channels become focusing features of high permeability within a slightly lower permeable sequences, effective for the advection of heat and mass (Hobbs 1987). This simplistic equation generated unrealistic features over a zone associated with high strain-rate in the thermo-mechanical simulation shown in the EPC 2 simulation. However, it may be proposed that this high-strain feature maybe an effect of total catastrophic rock failure before sagduction occurring within a short timeframe, such as the 10,000 year difference between EPC 2 and 3. Upon instantaneous brittle failure in seismogenic regions, large amount of fluids could have flowed through those damage zones. The magnitude of the amount of fluid was estimated to be at least 80% of fluid flow within the first three years of healing from hydrothermal fluids (Micklethwaite et al. 2015). The high geothermal gradients present in the Archean eons are capable of creating overpressurised fluids trapped under low-permeability seals. Any seismological induced enhancements in permeability would aid the release of that fluid pressure within a short period of time (e.g. Sibson 2004, 2002).

The overall stability of the fluid regime is highly dependent on the permeability field even in a generic conductive metamorphic setting, as seen in the progression of the sagduction process. This reinforces the significance of estimating permeability correctly in any generic fluid flow simulation.
4.5 Chapter Summary

Several fluid simulations were undertaken to understand fluid flow processes in a complex sagduction process set in a generalised granite-greenstone terrane. This was achieved through a one-way coupling of results from Ellipsis3D to SHEMAT. The permeability field in SHEMAT was evaluated through a depth-dependent permeability function and a linear alteration of strain-rate. A conservative linear relationship was established based on the merits of resultant fluid flow and thermal gradient.

As the process of sagduction matures with the growth of the thermal anomaly, the bulk of the fluids were observed to originate from the keel of the greenstones. Fluid fluxes achieved a maximum of $5.51 \times 10^{-5}$ m.s$^{-1}$ in EPC 4 (Fig 4.9). If the fluid contains a peak gold concentration of 0.65 ppm at $350^\circ$ C and fluid-rock interaction is 100% (Shenberger and Barnes 1989), the time taken for fluid to transport 1 MOz of gold will take in the 15th order of magnitude number of years. Such an astronomical number of years suggest fluid fluxes is not capable of transporting sufficient fluids to make a sizeable deposit. As mentioned in the previous sections, these high fluid fluxes were found in lower permeability regions or in close proximity with high heat sources at the lower crust. High fluid fluxes suggest fluid overpressure (e.g. Sibson 2004) and the hydrodynamic conditions around these regions were not suitable for any fluid convection. As soon as conditions for fluid convection are met, the fluids begin to thermally equilibrate through the expansion of energy via convective currents or via fluid-fracture propagation (e.g. Thompson and Connolly 1992). This first order approximation in developing strain-enhanced channels provides a solution in allowing Au-rich fluids to flow towards the surface.

The workflow has allowed the development of strain-enhanced channels useful for the focusing of fluid flow, providing the network to transport fluids throughout the greenstone and the surface. This method allows us to numerically evaluate how 'dynamic permeability'
could lead to further reinforcement of the fluid dynamic concepts caused by the ever-changing
dynamic conditions, improving our overall understanding of mineral systems.
Chapter 5

Conclusions

Results from these numerical experiments enabled the visualisation of high strain zones as suitable fluid pathways for fluid circulations. However, although this novel approach permits the simulation of fluid convection during crustal deformation while evaluating loci for hydrothermal mineralisation, a number of model limitations need to be highlighted and are presented in this final chapter.

5.1 Model Limitations

The modelling effort was limited due to the number of potentially unrealistic assumptions required to produce the simulations.

The first assumption is that of the model being saturated in fluids during simulation. This would be unrealistic. In a natural system, water is capable of reducing melting points (≈ 800° C for anhydrous minerals decreased to 670° C). Partial melting would occur at shallow depths (Phillips and Powell 2009. The initial temperatures of EPC 1 and 2 at the depth of 10km was below 400° C with little deformation experienced that is capable of producing metamorphic fluids from low-grade metamorphic rocks (Etheridge et al. 1983). However, if the initial thermal conditions are suitable for generating metamorphic fluids from dehydration
reactions, the fluid regime presented in EPC 1 (Fig 4.5 and 2 (Fig 4.7) may be correct. These limited fluids will converge with peak fluid flux identified in EPC 2 in Fig 4.7 (B) at the base of the greenstone cover. This leads to the second assumption where fluid simulation for each Ellipsis time step is independent to another Ellipsis time step.

The third assumption is about the properties of the fluids present in the model. The simulation considers the fluids as having the thermal and physical properties of water at standard temperatures and pressure. SHEMAT update fluid properties according to varying pressure and temperature conditions (Clauser 2003). The fluids which SHEMAT evaluates assume the thermal and physical properties of water. However, the pre-built routines in SHEMAT cause the simulation to overestimate fluid pressure and temperatures, leading to a decrease in accuracy near the critical point of water surmounting to probable numerical errors. The numerical code is limited to pressures and temperature below 100 MPa and 1000\°C respectively. In the case for the simulations conducted in this dissertation, the maximum temperature was around 850\°C which is still under the stated limitations of the numerical tool. Therefore, we need to take care in the interpretation of the results as a precaution of SHEMAT to overestimate pressure and temperature effects. In addition, the assumption of simulating pure water is also inaccurate as hydrothermal fluids usually contain large amounts of hydrous salts and minerals. These salts will affect the density thus influencing the fluid regime. A parameter sweep and sensitivity analysis is required to ascertain the effect of density on the fluid flow regime.

The fourth assumption is the initial driving force of hydraulic heading. Hydraulic head is evaluated by assuming the datum is at the base for each model, giving a constant value to all models. However, in reality, hydraulic heading might become over or under-estimated due to the shifting of the arbitrary datum. As a result, fluid flow influenced by hydraulic head may not be identical to the natural world processes. A further sensitivity study is therefore required to ascertain the appropriate level of hydraulic heading. Notwithstanding, the influence of
gravity induced hydraulic head on the resultant fluid regime is said to be minimal due to the
evaluation of Darcy’s Law. Darcy’s Law is primarily computed by hydraulic gradients and
any change in hydraulic heading seen in changes of topography is minimal (up to 3 orders of
magnitude (e.g. Cox 2001)). This effect pales into comparison with permeability (up to 12
orders of magnitude, discussed in Chapter 2).

The fifth assumption is about to the thermal and boundary conditions of the simulation. Each simulation has been constructed to assume to generic conductive metamorphic province only to be heated from a long heating source (a hotter lower thermal boundary) and are self-contained (impermeable fluid boundaries). The rocks and fluids were also assumed to lack the capacity to replenish their heat content (Chapter 2). Although these assumptions grossly simplify the conditions of natural systems, the fluids became more sensitive to thermal gradients imposed from the geodynamic setting.

The sixth assumption is the validation of strain-rates computed by Ellipsis. The correlation function enabled the evaluation of dynamic permeability through the reproduction of spatial representation of high strain zones. Consequently, these evaluated high strain-rate zones with permeabilities above $10^{-15} \text{ m}^2$ were observed at the base of the keel (up to the depth of 27 km) which are not realistic in the natural world. Lithostatic pressure at depth is capable of nullifying any potential fracture enhanced permeability (e.g. Rutqvist 2015). Strain-rate was evaluated from Ellipsis on the assumption of a function of strength of the lithosphere and depth (O’Neil et al. 2006). This function indicates the cold lithosphere at shallow depths exhibits high viscosity whereas a hotter lithosphere will exhibit lower viscosity. It is inferred that the higher strain-rate values at depth might be over-estimated as a consequence to the viscous deformation of the lithosphere. However, validating strain-rates at depth will be a challenge and can be investigated for further research.

When simulating SHEMAT models, great care had been taken to ensure minimal numerical errors. The criteria variables used by SHEMAT were checked to ensure their values
are kept as low as possible. However, in the high strained models seen in this chapter, the permeability and thermal conditions encourage fluid convection resulting in high \( Pe \) numbers. Higher \( Pe \) number infer higher thermal gradients up to \( 40^\circ \text{C/km} \) when \( Pe = 40 \) could consequently lead to the generation of erroneous temperature results (Bickle and McKenzie 1987). Shorter time steps were taken (up to 1000 years per period) with longer iterations (50 iterations per period) in an effort to decrease the value of these criteria.

## 5.2 Fluid flux thermal barrier conundrum

A recurring feature presented in all models is the substantial decrease in fluid flux (up to 2 orders of magnitude decrease) after breaching a certain temperature threshold (i.e. \( \sim 100^\circ \text{C} \) temperature contour). Streamlines in these areas indicate the presence of local circulations through the production of convection currents) to full convective cells. The fluids from the base were empowered by the high temperatures (up to \( 800^\circ \text{C} \)) allowing fluids to increase in pressure. These thermally enhanced fluids will be able to flow to the surface in higher speeds (up to a maximum fluid flux of \( 10^{-4.5} \text{ m.yr}^{-1} \)). According to Bickle and McKenzie [5], these high-energy fluids are capable of transporting massive amounts of mass and fluids in metamorphic rocks leading to potential economic deposits.

Fluid flow at depth is largely driven by gravity-induced hydraulic heading, leading to advective flow if \( Pe \) values are estimated to be over 2.0. Convective flow forces at depth were considered weaker than the initial gravity-induced hydraulic flow. The tug of war between gravity-induced and convective flow is further complicated with the medium’s permeability regime. For isotropic permeability models, we often evaluate \( Ra \) to determine the model’s hydrodynamic conditions. However, in an anisotropic permeability setting, a proper calculation of \( Ra \) using averaged permeability values is not feasible due to a 'logarithmic bias’ towards the larger values of permeability. Fluid convection began at a certain temperature threshold (\( 40^\circ \text{C} \) in models in Chapter 3 and \( 100^\circ \text{C} \) in EPC simulations) seen as the onset of local
Fig. 5.1 Schematic diagram for generic fluid activity in a generic conductive metamorphic setting at steady-state conditions. Gravity-induced dominant flow at depth flow towards the fluid-velocity thermal barrier. The fluids were observed to undergo convection around the fluid-velocity thermal barrier. As the fluids traverse past the barrier, additional circulation can occur if convective conditions persists.

circulations. If permeability conditions after that threshold are permissive for convection, these fluids will continue to convect. The presence of the convection currents is therefore suggested as a state of thermal equilibrium to the rest of the model.

5.3 Consistency of fluid flow patterns at lower influence of strain-rate to dynamic permeability

Our approach in performing a one-way coupling of strain-rate to evaluate dynamic permeability is capable of creating strain-induced channel networks at depth. As mentioned in Section 4.2.4, our local sensitivity analysis concluded that using $c = 2.5$ is a reasonable trade-off between resultant fluid activity and geothermal gradient. High and low fluid patterns are observed and the locality of convection currents occur in the lower flux regions. Higher fluid flux is described as gravity-induced hydraulic flow and have not met the conditions for
convection. By altering the value of \( c \) to 3.0, we would like to explore whether the fluid flow patterns are consistent with EPC 3 simulation.

In Fig 5.2 (A), EPC 3 at \( c = 2.5 \) displayed regions of high and low velocities. Convection currents were observed within the lower fluid flux region above the fluid-flux thermal barrier (black arrows). Unidirectional fluid flow occur within the higher fluid flux region, below the fluid-flux thermal barrier. When \( c \) was altered to 3 (Fig 5.2, the fluid-flux thermal barrier was observed to move up to 3 km below the surface of the greenstone block. The fluids were undergo convection after the fluid-flux thermal barrier (green arrow) indicating conditions for fluid convection were met and convective flows overcome gravity induced-forces. We infer that by raising the value of \( c \) causes fluid convection to decrease in intensity (based on size and quantity of convection cells), leading to a homogenisation of strain with our pre-defined permeability field. However, the resultant fluid activity seen in Fig 5.2 (B) was observed to be consistent by having gravity-induced flow in higher fluid flux regions and the possibility of convection cells in lower fluid flux regions.

5.4 Determining possible Au mineralising patterns

Before applying the RAI and the constrains from Chapter 3, the suitability of the EPC simulations for gradient reactions were assessed. These simulations are judged on the initial thermal gradients (shown in Fig 4.3), likely sources of fluids and the presence of convection currents. The greenstones in the thermo-mechanical experiment was assumed to be situated below sea-level, which heavily suggest the presence of an infinite fluid reservoir for possible downwelling of fluids (Thébaud and Rey 2013). The second source of fluids was derived from fluid release from the dehydration reactions of sagducting greenstones. The lowest temperature required to generate metamorphic fluids requires at least 400\(^\circ\) C. The presence of convective cells generated from the fluid flow regimes will determine local circulation, an agent to improve Au concentration at depth (e.g. Walshe and Cleverley 2009). The
Fig. 5.2 Comparison of fluid activity of EPC 3 simulation under different values of c. (A) represents the streamline and fluid flux magnitude plot of EPC 3 shown in 4.7 (B). (B) represents the streamline and fluid flux magnitude plot for EPC 3 when $C = 3.0$. Black arrows indicate presence of convection cells. Fluid advection occurs before the fluid-velocity thermal boundary (discussed in 5.1 before undergoing convection.

The evaluation of $RAI_{Au}$ suggests their sensitive nature to thermal gradients founded on gradient reactions (Zhao 2000, Phillips 1991). Convection currents are suggested to form regions of mineralization and mobilization of equal size shown in Fig 4.8 and Fig 4.9. Based on this temperature sensitive criteria, EPC 3, 4 and 5 simulations are possible candidates for metal gradient reactions.

$RAI$ was applied to EPC 3 simulation (Fig 5.3, EPC 4 and 5 simulations (Fig 5.4). Convection currents were identified (black arrows) and they correspond with equal regions of mineralisation and dissolution for $RAI$. This was the case in EPC 3 (Fig 5.3) but not for EPC 4 and 5 (Fig 5.4). Convection currents in EPC 4 and 5 were found at the fluid-velocity thermal interface discussed previously.

To reiterate, the use of $RAI$ and its expanded counterpart is good in identifying areas for gradient reactions. The only limitation is the sensitivity $RAI$ has with thermal gradient which is an oversimplification of a gradient reaction analysis. Additional information are required in
finding potential targets for exploration such as the presence of convection currents, general movement of fluid (upwellings and downwellings) and identifying for potential sources of fluids (i.e. percolation of seawater in a flooded continent setting (e.g. Thébaud and Rey 2013, Flament et al. 2008, Kump and Barley 2007)) or the mobilisation of sulphide-rich fluids through devolatisation (e.g. Tomkins 2010) as well as considering detailed physical and chemical fluid-rock interaction processes responsible for the deposition of the metal in solution.

## 5.5 Effect of lateral heat gradient to encourage convection currents

This dissertation was first established to evaluate high lateral thermal gradients into creating efficient fluid flow and associated fluid-rock interactions from a recent thermo-mechanical experiment (Thébaud and Rey 2013). These high thermal gradients were a consequence of the advection of hot rocks into rising domes in excess temperatures to 750°C, seen in 4.2. High lateral gradients were seen to be possible drivers of fluid from either the emplacement
Fig. 5.4 RAI workflow implementation with streamlines in EPC 4 (A) and EPC 5 (B). Black arrows represent localized fluid circulation. Colour bar show relative potentials in identifying high and low $RAI_{Au}$ values. Fluids is interpreted to offload its Au content as a function of decreasing thermal gradient. The absence of convection currents at these locations suggests no concentration of Au needed to form a deposit.

of plutons (e.g. Norton and Knight 1977, Eldursi et al. 2009) or the onset of sagduction (Thébaud and Rey 2013). However, fluid flow seen in the local sensitivity analysis (4.4) reinforces the significance of permeability. The less restrictive the resultant permeability field, the greater potential for the generation for convection currents, inspite of the greater potential of getting numerical errors.

Although the fluid flow regimes were analysed with streamflows and velocity (Fig 4.5 to Fig 4.10), there is a need to explore the correlation between thermal gradient and the fluid’s ability to undergo circulation. This concept of fluid flow being driven by lateral thermal gradients was postulated, especially around heat sources such as an intrusive pluton (e.g. Eldursi et al. 2009, Norton and Knight 1977). In Fig 5.5, plots for all simulations contain the resultant horizontal fluid velocity and the initial thermal gradient generated from Ellipsis at the depth of 10 km. These velocity values were taken as steady state solutions, to be consistent with the models presented in this chapter. This allows the possible mapping of
convection currents that were identified with each horizontal fluid velocity peak and trough suggested by Eldursi et al. (2009). Smaller deviations in horizontal fluid flux can be seen as the formation of convection currents. The scale at which velocity peaks and troughs were identified is model specific since their dimensions and geodynamic conditions were different.

Overall, the lateral thermal gradient can be seen as a precursor to the onset of convection (Fig 5.5). This is seen with large variations in thermal gradients in EPC 1 for the first set of convection current (EPC 1 in Fig 5.5). Smaller thermal gradients led to small deviations in horizontal fluid flux. This pattern can be translated to other models with the exception of EPC 4 (Fig 5.5). Thermal gradient was negative whereas horizontal fluid spiked at 4.0e-09 m.s\(^{-1}\) indicating high flux in upwelling of fluids. This was located at the permeability interface separating the greenstone and granites. The sudden improvement in rock permeability from strain is capable of improving conditions to encourage fluid convection. At EPC 6 (Fig 4.10), the sagduction process has completed and the level of variance in thermal field has reduced significantly. At 10 km depth (Fig 5.5), convection cells were present near the flux thermal barrier. The negative horizontal fluid velocity suggests downwelling is more prevalent. By comparing fluid movement in Fig 5.5 (A), downwelling flow was present at the left side and upwelling flow occurred at the right side of the keel.

### 5.6 Ellipsis and SHEMAT temperature fields problem

A comparison between the Ellipsis and SHEMAT temperature fields was attempted to understand the drastic change in temperature fields to Ellipsis (Fig 5.6). The range of differences is from \(\sim 100^\circ\) C from EPC 1 to a maximum of \(\sim 500^\circ\) C from EPC 4, 5 and 6.

This is caused by at least two effects, which were factored in to mitigate the loss of heat in the SHEMAT temperature field. The first consideration is establishing the relationship of \(C\) in determining dynamic permeability. \(C = 2.5\) was chosen to have a balance of fluid activity and resultant geothermal gradient. The higher the value of \(C\), the lower the permeability, the
Fig. 5.5 Initial lateral temperature gradient (Blue) plotted against horizontal component of fluid flux at 10 km depth for each EPC simulation. The arrow pairs indicate the presence of convective cells.
less active the convection currents and therefore the greater the resulting geothermal gradient. This leads to the second effect. Despite our best efforts in adjusting the value of dynamic permeability, the SHEMAT code to the difference to the Ellipsis code only allows boundary thermal conditions to be input in the simulation. For instance Ellipsis code is able to simulate the temperature field resulting from radiogenic rock decay in addition to the basal heat flux. SHEMAT does not allow for such heat source and since the fluids present in the system are not capable of producing their own heat the simulation evolves as a closed system that consumes the heat as fluid convection proceed. This effect is a direct consequence of the non-fully coupled method presented in this study.

5.7 Considerations for future work

The limitations identified during our experiments outline a framework for future work.

The first challenge is to examine the influence of strain-rate to rock permeability. Our approach was adopted to overcome the discussed limitations set by the numerical codes. A logical extension would therefore be to use a fully coupled thermal-mechanical and chemical approach. Our approach may be flawed as, data and models that describe the change to rock permeability by strain-rate are non-existent. However, based on the results presented in this dissertation, there can be merits on capitalising the speed of fracture formation and fracture sealing and/or healing (e.g. Cox et al. 2001). Our approach can also be validated through a detailed sensitivity analysis that can quantify the effects of uncertainty and entropy (e.g. Wellmann and Regenauer-Lieb 2012, Wainwright et al. 2014)

The next set of considerations is to explore the sagduction process in 3D. Although this dissertation endeavours to cover all considerations in 2D, some complexities remain unexplored that would be exposed using a 3D approach. By adding the extra dimension, it will ensure that the interpretations remain consistent and validates our approach. Our
Fig. 5.6 Difference in temperature fields at the depth of 10 km from two numerical codes. Blue line is the initial temperature field generated from Ellipsis. Red line is the resultant temperature field from SHEMAT.
numerical tools (Ellipsis and SHEMAT) are capable of rendering these models in the 3rd dimension.

The last set of considerations is to apply other solubility functions of other metals (Cu, Ag or Zn) and compare it with other published numerical techniques and mineralising systems. So far, the simulations have applied solubility function of Au. This would continue to validate our approach and is capable of creating an additional tool for researchers and industry alike.

In conclusion, the interplay of fluid flow, heat gradient and rock permeability remains to be very complex. Our novel approach in simulating the temporal aspect of deformation has enabled a greater appreciation to the nature of fluid self-organisation. This has profound implications to the mineral systems approach advocated by McCuaig and Hronsky [62] in determining ore deposit fertility in a generic Mesoarchean granite-greenstone terrane in a given geodynamic setting.
References


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Chapter 5


