Dynamic Modelling of Physical Processes in Magmatic Systems: Dyke Emplacement and Flow-Induced Crystal Rotations

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The main motivation for this thesis is to develop and improve numerical tools and methods that help further our comprehension of the volcanic plumbing system and its dynamics.

The commonly used standard elastic model predicts solutions of dyke shape, thickness, over-pressure and fracturing criteria that do not always fit natural observations. In the first part of the thesis, we want to test whether other host-rock rheologies leads to more realistic dykes. We examine three different rheologies: 1) elasticity with pressure dependent elastic moduli, 2) elastoplasticity with plastic failure in regions of high shear stresses and 3) viscoelasticity to describe ductile flow of rocks by creeping mechanisms in regions of high temperature. Solutions from the three tested models give dykes with more rectangular shapes relative to solutions computed from the model of linear elasticity. In addition, the calculated magma pressure for an intrusion of a given thickness is reduced for all tested rheologies. Greatest differences with the linear elastic solution are given by the elastoplastic model, in which computed magma overpressures are lower than elastic solutions by a factor of 2 to 10. Computed overpressures from this type of rheological model are approximately of the same order than natural magma overpressures estimated by other methods (1 to 5 MPa). For the model of dyke propagation, the incorporation of brittle failure mechanisms in regions of high stresses strongly affects the dyke propagation criteria because of the energy dissipated by frictional sliding and fracturing in the large process zone located at the intrusion tips.

The second part of the thesis deals with the rotation of crystals suspended in magmatic flows. We proceed by coupling the rotation dynamics equation of elongated particles, with the Navier-Stokes equation of large-scale flows. The results of the model are first extensively tested for simple flows with known analytical solutions. Results show a perfect fit between both numerical and analytical solutions. Additionally, the numerical methods are applied to more complex flow fields that relate to realistic systems of magma circulation. Results show that elongated crystals mainly align in the direction of flow in convergent systems (e.g. magma flowing from a large reservoir inside a conduit or from a deflating magma chamber). However, the pattern of crystal orientation in divergent flows (e.g. magma flowing from a conduit into a large reservoir or in an inflating magma chamber) does not align in the direction of the flow but instead is globally oriented sub-parallel to the maximum principal strain.

**Keywords:** Numerical solutions, elasticity and anelasticity, fracturing, magmatic plumbing system, sheet-like intrusions, rheology of the crust, physics of magma, solid mechanics, fluid flow, crystal rotation

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This thesis is dedicated to my family and friends.
List of papers

This thesis is based on the following papers, which are referred to in the text by their Roman numerals.


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1. Introduction

Volcanic eruptions are undoubtedly one of the most spectacular natural phenomena observed at the surface of the Earth. It is therefore not surprising that volcanism is and has been the focus of much research. Besides purely curiosity-driven investigations, there are also aspects of volcanology that are of high societal relevance. One such issue is the risk associated with volcanic eruptions. Every year an estimated 100 people lose their lives as a direct or indirect (mudslides, etc...) result of volcanic eruptions (Auker et al., 2013). Property damage in the same time frame is estimated around 150 to 200 millions EUR. Furthermore, the indirect consequences of volcanic eruptions can have a wide impact on our society. One recent example is the ash cloud associated with the 2010 eruptions of the Eyjafjallajökull volcano in Iceland, that caused a massive chaos in the air traffic all over Europe. Accurate forecasting of volcanic eruptions can reduce and perhaps eliminate those losses and consequences. With the present state of scientific methods, volcanologists are already highly successful at predicting eruptions, but nonetheless these methods can still be improved. The second aspect of volcanism that is of societal relevance is the economical benefit associated with the volcanic activity. Hydrothermal circulation is often caused by magma intrusion and associated fluids are channelized as a function of the geometry of the volcanic plumbing system, which locally concentrates various metals into high-grade ores. For example, we estimate that nearly all of the total ore production in Sweden formed as a result of hydrothermal activities. Geothermal energy utilizes the heat emplaced by volcanic intrusions. This heat can either be used directly, or converted to other type of energy. Currently, for example, Iceland generates 62 \% of its energy needs from geothermal sources. A third economical benefit of volcanism is the fertility of the soil that is often encountered in volcanic regions.

The focus of this thesis is on the development and improvement of methods and tools that aid in our understanding of volcano dynamics. The thesis comprises two parts.

In the first part, we study the inflation and the propagation of dykes and similar sheet-like intrusions. Mostly for reasons of simplicity, previous studies have assumed host-rock deformations to be linearly elastic. At high stresses and at high temperatures, it is well known that other deformation mechanism become dominant. We show that incorporation of brittle failure at high stress and viscous creep at high temperature significantly affect dyke shape, dyke opening and dyke propagation criteria such as fracture toughness.
The second part of the thesis deals with rotation of crystals or other rigid inclusions embedded in magmatic flows. It has long been known that elongate crystals not only rotate about their own axis, but, depending on the details of the flow, may also align themselves into a coherent pattern. In solidified magma flows, these alignment patterns are observable either directly in thin-section, or indirectly by techniques such as measurements of anisotropy of magnetic susceptibility (AMS). If the dynamics of crystal rotation and alignment are fully understood, than the observed alignment patterns serve as indicators of the velocity field of the flow. We extend the forward modelling of crystal rotations from homogeneous flows to flows that vary in space and time by coupling the rotation dynamics to the Navier-Stokes equation of the large-scale flow. Additionally, we introduce a differential equation for the evolution of the probability density function (PDF). After extensive testing, we apply the new method to a number of simple flows examples in order to provide insight on how realistic flow patterns affect crystal alignment.

In paper I, we numerically model the inflation of a two-dimensional sheet-like intrusion (dyke or sill), embedded in a continuous host-rock. At the beginning of the computation, the intrusion is defined by a nearly closed fracture that later open under the influence of a pressure condition applied on its inner boundaries. The thickness profile of the inflating fracture will then depends on the magnitude of the pressure condition and on the rheology (the deformation and flow behaviour of a material under an applied stress) of the surrounding rock. We therefore test three different rheological models, all based on the linear elastic model, although we allow for realistic host-rock rheology and map out their effects on the calculated fracture’s thickness profile. In the first model, the elastic moduli of the fracture’s wall-rock are pressure dependent to account for the formation and closure of microcracks, voids and pores in regions of tensile and compressive stresses. In the elastoplastic model, we take into account failure of material by fracturing and frictional sliding in the region of high shear stresses. Finally, in the viscoelastic model, we test the effect of ductile flow of the rock by creeping mechanism in region of high temperature. Our results show significant effects of the three tested rheologies on the calculated dyke geometries and pressure. For example, for a given fracture thickness profile we show that the pressure required for the elastoplastic model to fit the data is 70 to 90% lower than the pressure solution of the linear elastic model.

In paper II, we calculate the energy balance of a propagating fracture embedded in an elastoplastic host-rock and compare our results with the linear elastic solution. Our modelling methods are similar to those in paper I except that the fracture is not only inflating but also propagates from its tips. In this study, two types of fracture propagation are tested. In the first one, the propagation is done by continuous fracturing of the rock (propagation model), while in the second model the fracture evolves by successive episodes of in-
flation and incursion of magma in a pre-existing plane of weakness (inflation model). Our results show that plastic deformation impedes dyke growth in the propagation model, while it enhances dyke growth in the inflation model. The apparent fracture toughness computed from the elastoplastic propagation model, shows values that are $10^{-100}$ times lower than for the linear elastic model but of similar magnitude to fracture toughness measurements obtained from laboratory experiments.

In paper III and paper IV, we map out the preferred orientation of elongated crystals suspended in viscous flows. The objective of paper III is the development of a computational method to calculate the effect of the flow motion on the rotation evolution of suspended crystals. The local velocity field is decomposed into individual components, with each component having a distinct effect on the inclusion rotation. Inclusion orientations are given by a statistical probability density function that locally indicates the net orientation of a large crystal ensemble. To test our methods, we compute the preferred orientation of elongated particles along one stream line of a Couette flow, Poiseuille flow and corner flow. We then compare our results against known analytical solutions and show that our method agrees well with those solutions. In paper IV, we applied our computational methods to two-dimensional flows that relate to more realistic systems of magma circulation: an inflating magma chamber, magma flowing from a large reservoir into a sheet-like intrusion (and vice-versa), and magma convecting in a large reservoir. Our methods provide a way to test a given hypothesis of flow (or flow dynamics) for given crystal orientation observations.
2. General background and context of the thesis

Before examining the context of the thesis in detail, a brief overview of magma transport in the Earth’s crust is provided and how this overview can facilitate the comprehension of the work in this thesis. To do so, we first provide a brief history and description of magma ascent mechanisms, followed by the presentation and definition of the different components of the volcanic plumbing system. The section concludes with some of the open-questions related to magma transport and volcano dynamics.

2.1 General background: The volcanic plumbing system

The mechanism of magma ascent is a long debated topic. In the 20th century, two end-member models were proposed to illustrate magma transport through the crust: diapirism that involves magma blobs ascending through heated and softened host-rock, and dyking that relates to magma transport through thin conduits and fractures (Clemens, 1998; Petford, 2003). The model of diapiric upwelling involves positive buoyancy forces as the exclusive engine for magma ascending through the surrounding crustal rocks, meaning that the upward motion is controlled by the density contrast between the magma and the wall rock. This model is still used nowadays but mostly applied to the upward migration and emplacement of large granitic bodies embedded in the Earth crust, or to describe the formation mechanism of salt domes and salt diapirs. While buoyancy forces are also an important component in dyking, it has been shown that magma pressure is the principal engine for the magma ascent (Clemens & Mawer, 1992). Nowadays, it is generally agreed that dyking is the main mode of transport by which magma traverses the tens of kilometres of rocks in the crust, from its source level to surface level (Clemens & Mawer, 1992; Petford et al., 1994; Clemens, 1998; Clemens & Petford, 1999; Scaillet et al., 1998; Clemens, 2003), forming a part of the so-called volcanic plumbing system.

The volcanic plumbing system is a large network of magma conduits and reservoirs underlying volcanoes (see Figure 2.1). It is the major framework for magma transport and storage through the Earth’s crust, from the mantle source toward the surface. Most of the magmatic material (around 90 %) never reaches the Earth’s surface, but solidifies at depth and stays embedded in the crust until erosion or tectonic events expose part of the structure.
(Tibaldi, 2015). Direct observations of palaeo-plumbing systems (Kavanagh & Sparks, 2011; Daniels et al., 2012) combined with the recent development of underground imagery techniques and geophysical methods (Tryggvason, 1984, 1986; Toda et al., 2002; Wright et al., 2006) have greatly improved our understanding of the magmatic plumbing system.

The different observational methods have shown that magmatic reservoirs, namely magma chambers, are large pools of partially molten rock, more precisely crystal mushes that consist of a liquid matrix containing a large portion of solid phenocrysts, microliths and wall-rock pieces assimilated during transport of the magma (Maaløe & Scheie, 1982; McKenzie, 1984; Gudmundsson, 1987; Marsh, 1989; Sinton & Detrick, 1992). The accumulation of material in magma chambers leads to an important increase in the magma pressure in the closed reservoir. Consequently, the high magma pressure may cause fracturing of the surrounding host-rock or inflation and propagation of pre-existing fractures, forming conduits in which the magma is carried toward the surface.
These magma conduits were often represented as cylindrical pipes, but field observations combined with surface deformation measurement and seismicity analysis in volcanic regions indicates that they are typically are thin sheet intrusions with a very low thickness in comparison to their length and width. These intrusions are mostly vertical or inclined, cross-cutting the crustal rock fabrics and bedding that they are going through. These types of intrusions are called dykes. Sills constitute another type of magma channel, but they differ from dykes in that they form horizontal layers embedded between the surrounding rock fabric and that they are concordant to the lithology (Billings, 1972; Hall, 1996; Best, 2013). At shallow levels, a small portion of the sheet intrusions are feeder dykes supplying volcanoes with magma and fuelling eruptions in active volcanic regions. Most of the sheet intrusions are confined to regions surrounding volcanoes, however they sometimes reach the surface resulting in fissure eruptions or sustaining individual volcanic vents (Mège & Korme, 2004). Cylindrical conduits also exists but are mostly present in regions of andesitic volcanism (Zellmer & Annen, 2008). We present the mechanism of dyke propagation and inflation in more detail in section 2.2 and 2.3.

While the recent evolution in geophysical methods helped to refine our understanding and view of the volcanic plumbing system, a lot of questions have arisen and are still debated in the scientific community. How are the different components of the magmatic plumbing system formed and emplaced? and how is the magma moving through this plumbing network?, are essential questions in volcanology and in the study of magma transportation. Many studies have shown the role of the stress field in the structuring of the plumbing network (see reviews from Rivalta et al. (2015) and Tibaldi (2015), and references within) and pointed out the effect of the stress field interactions with pre-existing fracture and faults or with rheological heterogeneities of the surrounding wall rock (Gudmundsson, 2002; Rivalta & Dahm, 2004; Kühn & Dahm, 2008; Maccaferri et al., 2010; Geshi et al., 2012). There are several parameters and mechanisms that enter into the calculation of the stress field but the role of each of these elements is yet to be understood. In addition, the study of magma flow is of major importance in volcanology because the motion of magma and its rheology will have a direct influence on the volume flow rate in the volcanic plumbing system and thus on the eruptibility and eruption style of the volcanoes above (Marsh, 1981; Scaillet et al., 1998; Takeuchi, 2004).

2.2 Dyking and rheology of the crust

Paper I focuses on the dyke inflation mechanism and testing the effect of the host-rock rheology on the shape and size of dykes. This paper relates to the fundamental question of how sheet intrusions form and how they affect the magma dynamics in the plumbing network. Note that dykes are mainly mod-
elled in this study but our results apply to any type of magmatic intrusion, such as inclined sheets and sills, as their formation mechanisms are identical to dykes. In this section we aim to describe the general context for paper I and define the motivations to analyse the geometry of dykes embedded in continental crustal rocks. We first provide a description of crustal rock rheology and the associated solid deformation equations that we use for computation of the different rheological models. We also present a brief overview on the inflation mechanism of sheet intrusions and describe the different observations and modelling studies that have been carried out concerning this topic.

2.2.1 Rheology of the Earth crust

It is generally established that crustal rocks behave like a linear elastic medium under low stress and strain conditions and over short time scales. When these conditions are fulfilled, the applied stress is linearly proportional to the resulting strain and follows the fundamental general equation of linear elasticity, also called the Hooke’s law. For an isotropic material:

$$\sigma_{ij} = \frac{E}{1 + \nu} \left( \varepsilon_{ij} + \frac{\nu}{1 - 2\nu} \varepsilon_{kk} \delta_{ij} \right)$$  \hspace{1cm} (2.1)

where $\sigma$ is the stress tensor, $\varepsilon$ is the strain tensor, $\delta_{ij}$ is the Kronecker delta, and $E$ and $\nu$ are the Young modulus and Poisson’s ratio, respectively. In an elastic solid, the strain induced is not permanent and only exists if the load exist, and upon removal of the load, the strain goes back to 0 and the deformed rock instantaneously recovers its initial shape and size.

When the conditions for elasticity are not met, then the rock rheology is more complicated. In the brittle regime and for high stress and strain, rocks are observed to fail either plastically or by fracturing and subsequent frictional slip on the newly created fracture surfaces. In this regime of deformation, a part of the strain is non-recoverable upon removal of the applied load, thus on microscopic scale the rock will be permanently deformed due to the dislocation of the crystal lattice of individual minerals (Lawn, 1993) or due to microcracking of the mineral matrix (Paterson & Wong, 2005). On a larger scale, brittle crustal rocks are permanently deformed due to brecciation and frictional sliding (Rudnicki & Rice, 1975; Rubin, 1993). In continuous mechanics, brittle failure is often modelled using elastoplasticity. The failure criteria of brittle rocks can be described by the Drucker-Prager or the Mohr-Coulomb formulation (Paterson & Wong, 2005). The Drucker-Prager and Mohr-Coulomb yield criterion are both pressure-dependent mathematical models to determine the occurrence of fracturing or plastic yielding of a material. The Drucker-Prager model has a cylindrical yield surface, while Mohr-Coulomb has a yield surface that is a hexagonal prism. Other than that, the two criteria are similar. In the Drucker-Prager formulation, the failure criterion depends on the first invariant
of the stress tensor $I_1$ and on the second invariant of the stress deviator $J_2$. It can be calculated as follow:

$$f(\sigma_{ij}) = \sqrt{J_2} - k + \alpha I_1 = 0$$  \hspace{1cm} (2.2)

where $\alpha$ is the pressure-dependence of the yield stress and $k$ a form of material cohesion. The Mohr-Coulomb method describes the behaviour of brittle material in response to shear stresses and normal stresses, noted $\tau$ and $\sigma$ in this case. The failure criterion in this model is described by:

$$\tau = \sigma \tan \phi + C$$  \hspace{1cm} (2.3)

where $\phi$ is the frictional angle of the material and $C$ its cohesion. Both formulations are commonly used in Earth sciences, especially in problems related to fracture mechanics. While the Drucker-Prager yield criterion accurately takes pressure-dependency into account, the Mohr-Coulomb model is numerically less robust in the treatment of intermediate stresses due to the corner of yield surface. In both models, intermediate stresses are treated differently but truth seems to be in between Drucker-Prager and Mohr-Coulomb (Paterson & Wong, 2005).

On long time scales and/or at high temperature, rocks are observed to flow as the result of various creep mechanisms (Ranalli, 1995). Creep in solid mechanics describes the ability of the rock to deform permanently under an applied stress. It is a major deformation mechanism in the lower part of the crust (ductile part) where temperature approaches the solidus of the rock. There are two major components of creep: diffusion creep and dislocation creep (Turcotte & Schubert, 2014). Diffusion creep is mainly dominant at low stresses and describes the deformation of crystals by diffusion of void in the crystal lattice. Dislocation creep is the dominant type of creep at high stress conditions, and results from the movement of imperfections in the crystal lattice structure. In the diffusion regime of deformation, the viscosity of the rock is Newtonian, and the strain rate is linearly proportional to the deviatoric stress tensor:

$$\dot{\varepsilon}_{ij} = \frac{\sigma_{ij}'}{2\mu(T)}$$  \hspace{1cm} (2.4)

where $\mu(T)$ indicates the temperature-dependent viscosity. It important to mention that a lot of material are described by a non-linear relationship between the stress and the strain rate. In the case of a non-Newtonian rheology, the stress relates to the strain rate by a power law formulation (Paterson & Wong, 2005).

### 2.2.2 Dyking

In this thesis we refer to dyking as the process that leads to the formation and growth of sheet intrusions (vertical dykes, inclined sheets, or planar sills) in the
Earth’s crust. Sheet intrusions are mode I tensile fractures driven by the effect of pressurized magma injected in self-induced fracture (Bahat, 1980; Gautneb et al., 1989; Gudmundsson et al., 2001) or in pre-existing planes of weakness (Delaney et al., 1986; Baer et al., 1994; Delaney & Gartner, 1997; Valentine & Krogh, 2006). Their dimensions and shapes strongly depend on the stress state and rheology of the surrounding host-rock as well as the pressure of the injected magma. The propagation of sheet intrusions is preferentially oriented perpendicular to $\sigma_3$, the minimum normal stress, as this orientation allows opening against the least resistance (Anderson, 1951). As mentioned in section 2.1, they form the primary path for magma transport in the crust and are one of the major structures that affect volcano dynamics. Their shapes and sizes are therefore important parameters that control the volume of magma transported toward the surface and potential eruptions.

To help visualize and improve our knowledge on dyking, the scientific community can rely on observational data collected from field observations (e.g. structural geology observations, analyse of flow fabric in frozen dykes), lab measurements and geophysical methods (magnetic susceptibility, magnetotelluric, gravity, GPS, InSAR, seismicity). Among the methods mentioned above, measurements of surface deformation (GPS, Insar), help to follow the evolution and pressure-state of magma reservoirs (intrusions or magma chambers) by measuring the variation of surface deformation associated with their inflation and depletion (Newman et al., 2001; Yun et al., 2006). These types of measurements show that magma pressure in sheet intrusions is typically of the order of 1 to 5 MPa, which is in accordance with values obtained from other methods based on dyke propagation observations (Spence & Turcotte, 1985; Karlstrom et al., 2009) and thermal considerations for long-distance dyke propagation (Jellinek & DePaolo, 2003). Geophysical imagery techniques are another powerful tools that can be used to look at embedded active sheet intrusions in their entirety and then estimate the shape and volume of magma-filled intrusions as well as their geometry and size in three-dimensions (Montgomery-Brown et al., 2010; Nobile et al., 2012). Combined with field observations of exposed sheet intrusions, it shows that dykes and sills are distinguished from laccoliths, diapirs or cylindrical conduits by their low aspect ratio, with a thickness much less than their width and length. Dyke thickness is generally observed to be more or less constant along the entire length of the dyke (Rasmussen, J., 1978; Hoek, JD, 1995; Maaløe, 1998; Kavanagh & Sparks, 2011), and sometimes disturbed by local variations due to the presence of heterogeneities in the surrounding rock: rheological contrast, density layering, presence of faults and fractures; or by local variation of the magma pressure (Gudmundsson, 2002; Rivalta & Dahm, 2004; Kühn & Dahm, 2008; Maccaceri et al., 2010; Geshi et al., 2012). Dyke dimensions are observed to be typically of the order of about a centimetre to several meters in thickness and between a few meters to several kilometres in length and width (Tryggvason, 1984, 1986; Toda et al., 2002; Wright et al., 2006).
In two dimensions and under the simple assumption of static conditions in a linear elastic medium, the opening of a pressurized crack, or sheet-like intrusion in our case, can be calculated from knowledge of the dyke length and the magma pressure (Timoshenko, 2001). In this mathematical model, the pressurized crack is found to have an elliptical shape in its horizontal cross section defined by a semi-major and minor axes \(a\) and \(b\). The solution that describes the thickness profile \(u_y\) of the fracture along the semi-major axis \(a\) is given by (Sneddon & Lowengrub, 1969):

\[
u_y = \frac{2(1 - \nu^2)\Delta P}{E} \sqrt{a^2 - x^2}
\]

where \(x\) is the position in space along the axis \(a\), \(\Delta P\) is the overpressure of the magma (equal to the difference between the magma pressure and the lithostatic pressure), \(E\) the Young modulus and \(\nu\) the Poisson ratio. Comparison of dyke dimensions obtained from the linear elastic model against field observations shows that dykes tend to be more rectangular in nature (Pollard & Muller, 1976; Kavanagh & Sparks, 2011; Daniels et al., 2012) and thus do not fit the ellipsoidal shape predicted by the elastic theory. In addition, equation 2.5 can be rewritten in order to estimate magma overpressures in magmatic intrusions if the dimensions of the intrusion and the elastic moduli of the host-rock are known (Kavanagh & Sparks, 2011; Daniels et al., 2012; Becerril et al., 2013; Kusumoto et al., 2013). The overpressure \(\Delta P\) is then calculated from the aspect ratio \(a/b\) of the intrusion as follows:

\[
\Delta P = \frac{E}{2(1 - \nu)} \left(\frac{a}{b}\right)^{-1}
\]

This analytical solution gives results that often compare well with magma overpressure values estimated by other means (Spence & Turcotte, 1985; Karlstrom et al., 2009), however some studies describe overpressures computed from the linear elastic solution that are much higher, sometimes a factor of 10—100 (Poland et al., 2007; Daniels et al., 2012).

The mismatch between the linear elastic model and natural dyke shape and overpressure shows that the model does not provide a good description of the rheological behaviour of rocks. One possibility to reconcile models and natural observations is to consider the inelastic mechanisms (described in section 2.2.1) that affect the host-rock in regions of high stress and strain, which is typically the case near the tips of mode I fractures. This type of analysis is computationally much more complex, and hence the effect of more realistic rheologies on dyke aperture and magma overpressure has, thus far, not been examined. The motivation for paper I is to fill that gap and reconcile solutions from models with natural observations of sheet-like intrusions.

In this contribution, we build three rheological models, all based on the elastic solution but we allow for more realistic host-rock rheology. We first
test an elastic rheology with elastic moduli reduced in region of low stresses to include the effect of void formation and porosity in tensile region and their closing in compressive area (Walsh, 1965; Henyey & Pumphrey, 1982). Second we take into account failure of material by fracturing and frictional sliding in regions of high shear stresses (Paterson & Wong, 2005). Third, we test the effect of ductile flow of the rock by creeping to consider the influence of high temperature regions on the formation and growth of sheet-like intrusions (Ranalli, 1995).

2.3 Dyke propagation and fracture toughness

In paper II we study the propagation of mode I fractures, with a focus on sheet intrusions, and we discuss the concept of fracture toughness and Griffith energy balance applied to rocks. This study is in line with the fundamental question of how magmatic intrusions affect volcano dynamics and aim to further our knowledge on the formation and evolution of the magmatic plumbing system. In this section we first provide a brief review on the notions of fracture toughness, stress intensity factor and Griffith energy balance, fundamental concepts that describe propagation of tensile fracture in any solid material. In a second part, we define the mechanism of dyke propagation and discuss the linear elastic fracture mechanic model (LEFM) applied to dyking and the problems associated to it.

2.3.1 Griffith energy balance and fracture toughness

The Griffith energy balance is a global balance of the energy uptake and energy release while a pre-existing fracture is extended by an infinitesimal increment of length $\partial a$ (Griffith, 1921; Irwin, 1957). For pressurized fractures such as sheet intrusions, the energy uptake is due to the stress applied on the edges of a pre-existing fracture, while the energy release is due to the formation of new free surfaces as well as the inelastic dissipation at the process zone. In this case, the Griffith energy balance can be written as follow:

$$F_{\text{tot}} = \frac{\partial W_b}{\partial a} - \frac{\partial U_e}{\partial a} - \frac{\partial W_{\text{dis}}}{\partial a}$$

(2.7)

where $a$ is the length of the fracture, $W_b$ is the boundary work due to opening of the fracture, $U_e$ is the elastic energy and $W_{\text{dis}}$ is the energy dissipated by inelastic deformations in the process zone. In three dimensions, each of the terms above represent the energy uptake or release divided by the surface increment $\partial S$ of the newly formed fracture, with $\partial S$ equal to $\partial a$ multiplied by $w$, the width of the fracture. As $w$ is a constant and does not change during the propagation process, the different surface energy terms are then simplified and
are instead given as energies per unit length. The resulting term $F_{\text{tot}}$ is thus the energy per unit length that is left for the fracture to propagate and thus create new surfaces. $F_{\text{tot}}$ is equal to $G_c$ when the equilibrium between stability and propagation of the fracture is reached, with $G_c$ being a critical value that describes the energy required by the crack to propagate. $G_c$ can be treated as a material property that should only vary as a function of the composition of the host-rock. Because of the difficulty to measure quantities such as surface energies, the practical application of the Griffith energy balance and measurement of $G_c$ is nearly impossible to do from direct observations, thereby the analysis of fracture propagation needs to follow a different approach.

Material fracturing can be treated based on the analysis of the stress state at a fracture tip, assuming a linear elastic medium for the surrounding host-rock and neglecting any kind of inelastic deformations during the propagation and inflation process (Lawn & Wilshaw, 1975; Hertzberg et al., 2012). In the framework of linear elastic fracture mechanics (LEFM), the propagation of a mode I fracture relates to the contrasting concepts of fracture toughness $K_{Ic}$ and stress intensity factor $K_I$. The calculation of a stress intensity factor was first developed by Irwin (1957) who based his work on the Westergaard (1933) stress solution of a narrow slit embedded in a linear elastic medium and subjected to tensile stresses. The solution of Irwin (1957) is valid at the crack vicinity. The stress intensity factor links with the stress field as follows (Lawn & Wilshaw, 1975):

$$\sigma = \frac{K_I}{(2\pi r)^{1/2}} f(\theta)$$  

(2.8)

where $\sigma$ is any of the stress components, $r$ is the radial distance from the dyke tip, $K_I$ is the stress intensity factor and $f(\theta)$ is a factor function of the angle $\theta$, with $\theta$ depending on the chosen stress component. In the limit of elasticity, the stress approaches infinity at the very vicinity of the fracture tips ($r \to 0$). To avoid that stress singularity, a small area of inelastic deformation is theoretically introduced at the crack tips where the stress state is calculated from the Dugdale (1960) or Barenblatt (1962) model of plasticity. In this context, a critical value of $K_I$ at which fracture propagation occurs, the fracture toughness $K_{Ic}$, can be calculated. In theory, the fracture toughness is a material property, like $G_c$, that describes the resistance of a material to resist fracture. It is constant by definition and independent of the fracture evolution. In the limit of LEFM, the fracture toughness of a material can be calculated from equation 2.6 and 2.8 in conditions that the fracture or dyke’s dimensions are known and assuming that inelastic mechanism (fracturing, frictional sliding) are constrained to a very small area around the tips.

The Griffith energy criteria $G_c$ and fracture toughness are both describing the resistance of a material to resist fracturing but are defined from two different approaches of fracture propagation analysis, with the first one based on energy analysis and the other one based on stress analysis at the fracture tips.
Assuming negligible inelastic dissipation due to plastic deformation at the process zone ($W_{dis} \to 0$), the critical Griffith energy term relates to the fracture toughness as follows (Lawn & Wilshaw, 1975; Unger, 2001; Hertzberg et al., 2012):

$$G_c = \frac{K_{ic}^2 (1 - \nu^2)}{E}$$

(2.9)

where $E$ and $\nu$ are the Young's modulus and Poisson ratio, the elastic parameters of the fracture host-rock.

### 2.3.2 Propagation of sheet intrusions in crustal rocks

In the brittle part of the crust, the propagation of dykes or sheet intrusions occurs either by continuous fracturing of the rock or by successive inflation and incursion of magma in a pre-existing plane of weakness. In the first case, the failure of the rock occurs at the tip of the intrusion where the stress concentrates because of the elongate geometry of the fracture and the narrow radius of curvature of its tips (Lawn & Wilshaw, 1975; Tada et al., 2000).

The direction of propagation of the magmatic intrusion is mainly affected by its external factors. Among the potential factors, it is generally considered that the effect of external stress sources on the intrusion's self induced stress state, is the major mechanism that influences dyke propagation direction. For example, the load of a volcanic edifice (Dahm, 2000; Gudmundsson, 2002; Watanabe et al., 2002; Maccaferri et al., 2011), the loading-unloading cycle of icecap (Albino et al., 2010; Hooper et al., 2011), the regional tectonic setting (Parsons et al., 1992; Kühn & Dahm, 2004, 2008; Maccaferri et al., 2014), are all mechanisms that alter the stress field around the intrusion and hence modifies its direction of propagation. Propagation of sheet intrusions can also be perturbed by the presence of heterogeneities in the surrounding rock. For example, it was shown that rheological contrast in the host-rock, the presence of pre-existing faults and fractures in the close vicinity of the intrusions and interactions with other sheet intrusions or magma chambers, are all possible sources of perturbation for the dyke evolution (Gudmundsson, 2002; Rivalta & Dahm, 2004; Kühn & Dahm, 2008; Maccaferri et al., 2010; Geshi et al., 2012). On the same subject, dyke arrest is a long debated question in volcanology and fracture mechanics. Why and how dykes or fractures are susceptible to stop propagate is yet to be answered. Some authors suggest that a stress barrier induced by volcanic loading (Dahm, 2000; Gudmundsson, 2002; Watanabe et al., 2002; Maccaferri et al., 2011) or density layering (Taisne & Jaupart, 2009; Maccaferri et al., 2011), can cause a dyke to stop its propagation. Magma solidification inside the dyke, faulting, pressure decrease in the magma chamber (Rivalta, 2010) and the change in the local stresses, are also good candidates to explain dyke arrest. As mention in section 2.3.1, the stability of a mode I fracture against fracturing can be predicted by
the fracture toughness of the surrounding medium. Within the LEFM model, fracture toughness of rocks can be estimated from aspect-ratio observations of exposed dykes, assuming that inelastic deformations are constrained to a very small zone located at the intrusion tips. In this framework, typical values of fracture toughness for crustal rocks are generally constrained between $50 - 200 \text{ MPa.m}^{-1/2}$ (Delaney & Pollard, 1981; Parfitt, 1991; Schultz et al., 2008; Kusumoto et al., 2013). In comparison, fracture toughness estimated from lab measurements on crustal rocks are estimated to be lower by almost a factor of 100, with typical values averaging $1 - 3 \text{ MPa.m}^{-1/2}$ (Balme et al., 2004; Zhang & Zhao, 2014).

The important disparity between both fracture toughness solutions mainly shows that assumptions behind the LEFM model are not valid for rocks. Indeed, it was shown from field evidences that rock failure and consequently inelastic deformation occurs in a broad zone that extends far from the dyke tips and often affects the wall rock along the intrusion edges (Rubin & Pollard, 1987; Kavanagh & Sparks, 2011; Daniels et al., 2012; Abdelmalak et al., 2012; Scheibert et al., 2017; Guldstrand et al., 2017). In this context, inelastic deformation in crustal rocks cannot be considered as a consequence of small scale failure constrained to a small area around the tips of the magmatic intrusion. Furthermore, in the small-scale failure regime, fracture toughness is assumed to be independent of the fracture geometry and length, so that it is considered as a material property. In reality, fracturing and frictional sliding affecting the dyke tips scale with the fracture dimensions and, moreover, the size of that damaged zone generally increases as a function of the fracture length and fracture aperture. These observations imply that fracture toughness cannot be considered as a material property but instead should vary in function of the intrusion or fracture length (Pollard & Muller, 1976; Vermilye & Scholz, 1995; Scholz, 2010). Hence, it is clear that inelastic mechanisms would greatly alter the fracture toughness of the rock around the dyke tips. Furthermore, the dependency of the fracture toughness on the fracture dimensions has already been shown from lab measurement.

In paper II, we study the Griffith energy balance of a propagating sheet-like intrusion for different host-rock rheologies. We mainly test an elastoplastic rheology (Paterson & Wong, 2005) and calculate the different Griffith energy terms (see equation 2.7) for a static dyke. By testing this type of elastoplastic rheology, we take into account the effect of large scale failure of the rock on the calculation of the Griffith energy balance. In this context, we expect non-negligible dissipated energy by inelastic deformation around the intrusion tips. We test two types of fracture evolution: 1) a sheet intrusion that propagates at constant overpressure and 2) a series of sheet intrusions inflating pre-existing fractures.
2.4 Magma flow and Crystal rotation

In paper III and IV, we investigate the rotation of solid particles suspended in viscous flows. The purpose of these two studies is to understand the pattern of crystal alignment in different types of basic flows (paper III) and in more complex active magmatic systems (paper IV). The objective of these two papers is to provide the link between field observations of crystal orientation in solidified magmatic intrusions with the history of the magma dynamics before its solidification. The motivation behind these two studies is to further our understanding on magma circulation in the Earth’s crust because of its direct influence on the dynamics of volcanoes. In this section, we first provide basic theory on the mechanism of crystal rotation in viscous flow and second, we provide a general knowledge about flow induced crystal alignment in solidified magmatic complexes.

2.4.1 Rotation of solid particles in viscous flows

Solid particles of various shapes and sizes rotate around their own axes when they are suspended in viscous flows. By neglecting particle-particle and flow-particle interactions, the rotation rate of the solid crystal can be calculated based on the description of the flow motion. A general approach to analyse crystal rotation suspended in a flow is to decompose the local velocity field into independent components. The first approach splits the flow into a simple shear and pure shear component, while assuming that volume changes are negligible (Jeffery, 1922). This approach is commonly used in the analysis of tectonic settings where large scale systems are subjected to pure and simple shear deformations, or to a combination of both components, namely transtension and transpression. Alternatively, we choose to split the velocity field of the flow into two components of pure shear and solid body rotation (Willis, 1977; Fung & Tong, 2001). In this case, the velocity vector \( v_i \) of the flow field can be written as the sum of a solid body translation \( v_i^0 \), a solid body rotation

\[ v_i = v_i^0 + u_0 \]

\( u_0 \) is the uniform translation, \( v_i^0 \) is the pure shear flow, and \( v_i \) is the total velocity.

![Figure 2.2. Decomposition of the velocity field for a Couette flow.](image)
rate $\omega_{ij}$, a rate of volume change $\dot{\varepsilon}_{ii}/3$ and a pure shear strain rate $\dot{\varepsilon}_{ij}'$ (see e.g. for a Couette flow in Figure 2.2).

The total rotation rate of a solid particle embedded in a flow can thus be written as the sum of the individual rotations rate due to the four flow components. For crystal with ellipsoidal shapes, the total rotation rate in a three dimensional-space will be (Jeffery, 1922; Jiang, 2007; Marques et al., 2014):

\[
\omega_1' = \dot{\omega}_{23}' + \frac{b^2 - c^2}{b^2 + c^2} \varepsilon_{23}' \\
\omega_2' = \dot{\omega}_{31}' + \frac{c^2 - a^2}{c^2 + a^2} \varepsilon_{31}' \\
\omega_3' = \dot{\omega}_{12}' + \frac{a^2 - b^2}{a^2 + b^2} \varepsilon_{12}'
\]

(2.10a,b,c)

where $a$, $b$, and $c$ are the three semi-axes of the ellipsoid and $\omega_1'$, $\omega_2'$ and $\omega_3'$ are the three total rotation rates of the particle around its three rotation axes. For most flows and crystal shapes, both translation and volume change terms are assumed to have no influence on the rotation of a particle. However, the solid body rotation and shear strain rate will exert a torque on the solid particle and cause its rotation. The right-hand side of the equation defines the rotation rate due to pure shear flow and is a function of the particle aspect ratio. The left-hand side of the equation defines the rotation rate due to solid body rotation and only depends on the velocity gradients of the flow such as:

\[
\omega_{ij} = \frac{1}{2} \left( \frac{\partial v_i}{\partial x_j} - \frac{\partial v_j}{\partial x_i} \right)
\]

(2.11)

In two dimensions and assuming negligible inertial forces in the system, the rotation rate of an ellipsoidal solid particle immersed in a viscous flow can be calculated as follows (Jeffery, 1922):

\[
\dot{\theta} = \frac{1}{2} \left( \frac{\partial v_y}{\partial x} - \frac{\partial v_x}{\partial y} \right) - \frac{1}{2} (\dot{\varepsilon}_1 - \dot{\varepsilon}_2) \frac{a^2 - b^2}{a^2 + b^2} \sin(2\theta - 2\theta_p)
\]

(2.12)

where $a$ and $b$ are the semi-major and semi-minor axes of the particle, $\dot{\varepsilon}_1$ and $\dot{\varepsilon}_2$ are the maximum and minimum principal strain rates of the two dimensional flow, $\theta$ is the angle of the solid particle with the horizontal axis, and $\theta_p$ gives the direction of $\dot{\varepsilon}_1$.

2.4.2 Magma flow

A magma in geology describes a plastic and hot material, more precisely molten rocks, containing dissolved gas and crystals. It forms at high temperature and under high pressure during the partial melting of crustal rocks.
in the Earth’s mantle. On short and long time scale, a magma can be defined as a fluid, characterised by a low viscosity value in comparison to rocks. For example, at a temperature superior to the rock’s liquidus, the viscosity of the magma is around $10^2 - 10^4$ Pa.s for a basalt and around $10^{10} - 10^{12}$ Pa.s for a rhyolite. In general, geological fluids such as magma carry solid inclusions in suspension, like pieces of wall rock assimilated during the ascending journey or phenocrysts and microlits formed during the cooling process.

It is commonly known that these solid particles of given shape and aspect ratio are not only advected along the magma flow, but additionally rotate around their own axes and sometimes align in the direction of flow. The rotation of the particle is mostly the consequence of the velocity field on the particle walls and the pressure perturbation at the vicinity of the solid particle (see Figure 2.3), which generate a torque responsible for the rotation (Marques & Cobbold, 1995; Marques & Coelho, 2001).

In Earth science, the study of particles and their rotation is critical. Indeed, the presence of solid inclusions will have a major influence on the rheology of the flow (Einstein, 1906; Roscoe, 1952; Kerr & Lister, 1991; Vigneresse et al.,

Figure 2.3. Pressure state around an elliptical particle of aspect ratio $a/b = 2$, embedded in a simple shear flow.

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Thus, for magmatic material, the concentration of solid particles in the liquid matrix will modify the flow pattern and hence the type of eruption of a volcano. Another reason to study particle inclusions is that the pattern of orientation of solid particles embedded in solidified magmatic systems can be seen as markers of the deformation. At a larger degree, magmatic inclusions and their patterns of orientation can provide indirect evidences on the magma dynamics for when the system was still active.

Observations of phenocrists and microlits in exposed solidified magmatic reservoirs show that elongated crystals are not randomly organized but mostly align parallel to the walls of the reservoir, with their longest axis (major-axis) oriented in the direction of flow (Smith, 2002; Paterson, 2009; Chistyakova & Latypov, 2010; Yamato et al., 2011). Moreover, it is observed that crystals are distributed throughout the solidified magma in function of their size, with biggest crystals located at the center of the reservoir and smaller ones located at the edges. All these observations are indicators of the relict magma flow pattern of when the system was still active. However, these indicators are only indirect evidences of the pattern of flow and only relate to the last increment of strain before solidification of the magmatic complex. A link between observational data and magma dynamics of the active system is thus difficult to make. To fill that gap and understand the relation between active flow field and crystal orientation observations, numerous analogue (Willis, 1977; Arbaret et al., 2001; Marques & Coelho, 2001, 2003) and numerical modelling studies (Bons et al., 1997; Mandal et al., 2001; Marques et al., 2005b,a; Yamato et al., 2011) have been carried out. The majority of those studies based their work on the Jeffery (1922) theory and are applied to the rotation analysis of ellipsoidal crystals embedded in homogeneous flows.

In paper III and IV, we extend this type of analysis to flows that vary in space and time (heterogeneous flows). To do so, we proceed by coupling the crystal rotation equation (Equation 2.12) with the Navier Stokes equation for flows. Additionally, we provide the orientation of crystals as a probability density function which describes the preferred orientation of a large crystal ensemble at every points of the tested flow. We first develop the theory of our methods and compare output with known analytical solutions and other results (paper III) and second, we apply our methods for more complex cases that relate to typical subvolcanic flows (paper IV).
3. Methods

3.1 Finite element methods

Throughout this thesis, we use finite element methods (FEM) to solve the governing equations of solid mechanics and fluid flow used in our modelling studies. The original laws of physics applied to those space- and time-dependent problems are generally expressed in terms of partial differential equations (PDEs) that cannot or hardly be solved by classical analytical methods. FEM are numerical tools that use mesh generation to subdivide a complex problem into smaller and simpler part called finite elements. The discretization of complex problems into small elements allow to approximate PDEs to numerical model equations and solve them using computational methods. Finite element methods can handle very complex geometries, constrains and loading conditions of a system and are used to solve a wide variety of engineering problems (solid mechanics, dynamics, heat transport problems, fluid flow etc...). Unfortunately, solutions from FEM are just approximating real solutions with an accuracy that depends on the resolution of the mesh system. Throughout this thesis, we used the commercial modelling software Comsol Multiphysics® (2017) coded with FEM algorithm, to solve the time and space dependent problems described in each papers. Comsol Multiphysics® (2017) is a numerical modelling software that can couple multiple physics at the same time (Fluid flow, heat transfer, solid mechanics etc...), and it contains several essential tools and features for our work (remeshing, ALE elements, stabilization of solutions, etc... ). The code has already been tested and benchmarking against known analytical solutions or other numerical softwares, thus a strong confidence can be given to the veracity of the results.

3.2 Solid deformation

The first part of the thesis (Paper I and II) focuses on the solid deformation associated with the inflation and propagation of a vertical magmatic intrusion (dyke). We use finite element methods to solve the linear stress-strain equation associated to the deformation of the dyke host-rock (Eq.2.1).

In our numerical models, solid deformation operates on two different set of coordinates: one defining the spacial frame of the physical domain Ω (noted \(x, y\) and \(z\) in 3-D and \(\mathbf{x}\) in vector form), and a second set known as the material frame and used to label material particles position (noted \(X, Y\) and \(Z\) in 3-D
and \( \mathbf{X} \) in vector form). By definition, both material and spacial coordinate systems coincide as long as the solid domain is undeformed. When applying a force (or a pressure condition in our case) on the solid object, the material coordinates \( \mathbf{X} \) are unchanged but the spacial coordinates become:

\[
x = x(\mathbf{X}, t) = \mathbf{X} + \mathbf{u}(\mathbf{X}, t)
\]

(3.1)

where \( \mathbf{u} \) is the displacement tensor. This equation can be described as the sum between the material position (reference frame) and the displacement caused by the pressure or force condition.

In its deformed state, the initial coordinates of a solid and continuous medium are displaced by some vectors \( u, v, \) and \( w, \) the \( x, y \) and \( z \) components of the displacement tensor. In three dimensions, the nine components of the deformed material strain tensor relate to the mentioned displacement vectors and can be calculated as follows:

\[
\begin{align*}
\varepsilon_{xx} &= \frac{\partial u}{\partial x} \\
\varepsilon_{xy} &= \varepsilon_{yx} = \frac{1}{2} \left( \frac{\partial u}{\partial y} + \frac{\partial v}{\partial x} \right) \\
\varepsilon_{yy} &= \frac{\partial v}{\partial y} \\
\varepsilon_{yz} &= \varepsilon_{zy} = \frac{1}{2} \left( \frac{\partial v}{\partial z} + \frac{\partial w}{\partial y} \right) \\
\varepsilon_{zz} &= \frac{\partial w}{\partial z} \\
\varepsilon_{xz} &= \varepsilon_{zx} = \frac{1}{2} \left( \frac{\partial u}{\partial z} + \frac{\partial w}{\partial x} \right)
\end{align*}
\]

(3.2a, b, c)

It is possible to simplify in two dimensions the three dimensional equations of strain and stress under certain assumptions of plane strain or plane stress. In plane stress problems, the piece of rock geometry is that of a plate with one dimension much smaller than the two others and with the principal stress in the smallest direction assumed to be 0. In this case the stress tensor is simplified and can be described by a tensor of dimension 2. In plane strain problems, the piece of rock geometry is that of an infinitely long column with one dimension much larger than the others. The principal strain in the longest dimension is then constrained and can be approximated to 0 while the resulting global strain tensor reduces to a tensor of dimension 2.

A Lagrangian formulation is used to discretize our solid deformation problems. Computed deformation and stresses are therefore always referring to the material coordinate system \( (\mathbf{X}) \) rather than the spacial position \( (\mathbf{x}) \). As a result, varying material properties in space are evaluated once at the initiation of the computation and do not change even if the solid domain is subjected to rotation and/or deformation.

### 3.3 Fluid flow

A lot of geodynamics problems relate to fluid mechanics, which is typically the case of magma transport and flow in the magmatic plumbing system (paper
III and IV). Fluid mechanics is a discipline that describes the motion of a fluid (liquid, gas, plasma) in response to an applied stress. The behaviour of a fluid in motion answers to fundamental equations, namely the conservation law of mass:

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{v}) = 0 \quad (3.3)$$

and the conservation law of momentum, here written for fluids in the Navier-Stokes form and for an incompressible and Newtonian flow:

$$\rho \left[ \frac{\partial \mathbf{v}}{\partial t} + (\mathbf{v} \cdot \nabla) \mathbf{v} \right] = -\nabla p + \rho g + \mu \nabla^2 \mathbf{v} \quad (3.4)$$

where $\rho$ and $\mu$ are the density and viscosity of the fluid, $g$ is the gravitational constant, $p$ is the pressure and $\mathbf{v}$ is the velocity vector. Term 1) describes the change in time of the fluid velocity, 2) is the convective term, 3) is the pressure gradient because fluid flows in the direction of largest pressure changes, 4) is the body forces term and describes the effect of external forces that act on the fluid and 5) describes the diffusion of the velocity, with the magnitude of the diffusion that depends on the viscosity of the fluid. The stress state in a flow is connected to the velocity gradients or to the rate of strain of the fluid elements by the rheological law of the fluid. The simplest flow is described by a Newtonian or linear rheology, where the strain rate is linearly proportional to the applied stress by the viscosity of the fluid $\mu$:

$$\sigma'_{ij} = 2\mu \dot{\varepsilon}_{ij} \quad (3.5)$$

and where $\sigma'_{ij}$ is the deviatoric stress tensor. There exist non-Newtonian types of flow, where the stress tensor is linked with the strain rate by a power-law formulation:

$$\sigma'_{ij} = 2\mu (\dot{\varepsilon}_{ij})^n \quad (3.6)$$

where $n$ depends on the rheology of the flow.

An Eulerian formulation is used in order to discretize the fluid flow problems presented in paper III and IV. The computational mesh is fixed in space and time and the material moves through the grid. The Eulerian formulation has the advantage to handle very large deformation and distortion of the continuum but does not allow deformation of the geometric domain.

### 3.4 The heat equation and temperature dependent density

In some of our dyke rheological models or fluid flow problems, calculation of the temperature field was required. The temperature field can be calculated by
solving the heat equation:

\[ \rho C_p \frac{\partial T}{\partial t} + \rho C_p \mathbf{u} \nabla T = \nabla \cdot (k \nabla T) + Q \]  

(3.7)

where \( \rho \) is the density, \( C_p \) is the specific heat capacity at constant pressure, \( T \) is the temperature, \( \mathbf{u} \) is the velocity vector, \( k \) is the thermal conductivity and \( Q \) contains heat sources different than viscous heating. The heat equation can also be written in function of the thermal diffusivity \( \kappa \) of the material with \( \kappa = k/\rho C_p \).

In paper I, one of the tested rheology is viscoelastic and thus viscous contribution to the wall dyke deformation required computation of the temperature field in the model domain. The heat equation is solved numerically and is coupled with the fundamental equations of solid deformation used in the dyke inflation model. We used thermal parameters that are typical for crustal rocks and magmatic material, with \( \kappa = 1.3 \times 10^{-6} \text{ m}^2\text{s}^{-1} \) and \( \kappa = 0.98 \times 10^{-6} \text{ m}^2\text{s}^{-1} \), respectively (Clauser & Huenges, 1995).

Paper IV involves a convection model, with the density of the viscous flow varying in function of temperature as follows:

\[ \rho(T) = \rho_0 [1 - \alpha (T - T_0)] \]  

(3.8)

where \( \rho_0 \) is the reference density of the material, \( T_0 \) is the initial temperature of the fluid and \( \alpha \) the expansion coefficient. For this type of model, the heat equation is coupled with the Navier-Stokes equation for a fluid. The following thermal parameters are used: \( k = 2.25 \text{ W.m}^{-1}\text{K}^{-1} \) and \( C_p = 750 \text{ m}^2\text{s}^{-2}\text{K}^{-1} \).

3.5 Numerical calculation of the Griffith energy terms

Considering a 2-D domain in plane strain of area \( A \) and intruded by a crack, the different terms of the Griffith energy balance presented in Section 2.3.1 are calculated in paper II from the following equations:

- The first term \( W_b \) is the energy uptake (boundary work) due to the inflating boundaries of the fracture. The boundary work along the fracture walls is analytically computed in Comsol Multiphysics following the equation introduced by (Lawn & Wilshaw, 1975):

\[ \delta W_b = \int_L \Delta \rho \mathbf{\hat{n}}_i \mathbf{u}_i \, dL \]  

(3.9)

where \( \mathbf{\hat{n}}_i \) is the unit vector perpendicular to the fracture wall, \( \mathbf{u}_i \) is the displacement vector of the fracture wall, and \( L \) indicates integration along the boundary of the fracture.
• The energy release due to the elastic deformation of the fracture surroundings is numerically solved as follows (Malvern, 1969):

\[ U_e = \frac{1}{2} \int_A \sigma_{ij} \varepsilon_{ij}^e dA \]  

where \( A \) is the area of the domain, \( \varepsilon_{ij}^e \) is the elastic component of the strain tensor and \( \sigma_{ij} \) the stress tensor.

• The work done by dissipation due to inelastic deformation (plastic or viscous flow) can be calculated using (Malvern, 1969):

\[ \delta W_{\text{dis}} = \frac{1}{2} \int_t \int_A \sigma_{ij} \dot{\varepsilon}_{ij}^i n dA \, dt \]  

where \( \dot{\varepsilon}_{ij}^i n \) is the inelastic component of the strain rate.

3.6 Probability distribution function and conservation law for crystal orientation

A probability density function is a function that describes the probability distribution of a variable \( X \) in an interval \([a − b]\) so that:

\[ Pr(a \leq X \leq b) = \int_a^b P(x) \, dx \]  

The probability \( Pr \) that \( X \) takes a value between \( a \) and \( b \) will be the grey area comprise in the interval and under \( P(x) \) the density curve (see Figure 3.1). A pdf answer to some properties so that the total probability integrates to unity and \( P(x) \) is always positive, 

\[ P(x) \geq 0 \]  

![Figure 3.1. Probability density function.](image)
\[ \int_{-\infty}^{+\infty} P(x)dx = 1 \quad (3.14) \]

Moreover, the probability for \( X \) to attain a single value is always zero,

\[ Pr(X = a) = \int_{a}^{a} P(x)dx = 0 \quad (3.15) \]

The probability density is different than a normal probability and \( P(x) \) can be superior to 1.

In paper III and IV, the particle angle between the rotation axis and the horizontal, namely \( \theta \), is given as a probability density function (PDF) defined between 0 and \( 2\pi \) and varying in space and time \( (P(x,y,t,\theta)) \). The PDF has the obvious advantage to provide a net or mean orientation of the particle, which is a more useful information for the analysis of large crystal ensemble than just providing the absolute orientation of a single crystal. Note that the PDF approach requires that all particles are identical, with the same shape and same aspect ratio.

In our two fluid flow studies, we assume that crystals and their orientations cannot be created nor destroyed, thus \( P \) should be conservative and its evolution in time can be described by a conservation equation of the form \( \partial P/\partial t = -\nabla \cdot (P \mathbf{u}) \) (Malvern, 1969), where \( \mathbf{u} \) is the velocity vector of the flow field. For a 2-D flow defined in a \( x-y \) Cartesian coordinate system, the crystal orientation and thus \( P(\theta, t) \) get advected by the flow. The evolution in time of \( P \) can be describe by:

\[ \frac{\partial P(\theta)}{\partial t} = -u_x \frac{\partial P}{\partial x} - u_y \frac{\partial P}{\partial x} - P \frac{\partial \dot{\theta}}{\partial \theta} - \dot{\theta} \frac{\partial P}{\partial \theta} \quad (3.16) \]

with 1) being the advection term in \( x \) and \( y \) of \( P \) in the physical space and 2) is the contribution of the differential crystal rotation at a fixed point of the flow.
4. Paper summary

4.1 Paper I: Effect of Host-rock rheology on dyke shape, thickness and magma overpressure

In paper I we aim to reconcile the long-term mismatch between dyke thickness, shape and magma overpressure observations (Spence & Turcotte, 1985; Newman et al., 2001; Jellinek & DePaolo, 2003; Karlstrom et al., 2009; Daniels et al., 2012) with solutions predicted by the widely used standard elastic model (Kavanagh & Sparks, 2011; Daniels et al., 2012; Becerril et al., 2013; Kusumoto & Gudmundsson, 2014). The standard elastic model predicts a dyke’s geometry to be perfectly elliptical in its horizontal cross-section, whereas dykes in nature are observed to be more or less constant over their length with a sharp taper at the end. In addition, computed overpressures to inflate dykes in a purely elastic medium are much higher than values estimated from other methods (see Section 2.2.2). In this study, we use 2-D numerical models to map out the effect of more complex deformation mechanisms on the geometry, dimensions and overpressure solutions of a dyke inflating in a continuous medium (host-rock), and we compare solutions with observational data collected from previous publications (Daniels et al., 2012). We test three different host-rock rheologies: 1) An elastic rheology with elastic moduli reduced in regions of low pressure, 2) an elastoplastic rheology to take into account failure and frictional sliding in the host-rock (mostly localised in the process zone surrounding the crack tips) and 3) a viscoelastic rheology that reflects rock ductile behaviour in regions of high temperature.

4.1.1 Modelling approach

We use the same modelling approach for the three tested rheologies and aim to compute dyke thickness profiles of static dykes (no pressure gradient and no inertial forces) submitted to magma overpressure.

The model domain consists of a 2-D box that is 10 km × 10 km in dimension with no-slip boundary conditions at its edges. To account for the third dimension, we employ an axisymmetric symmetry that is appropriate for a perfectly circular dyke in its two longer dimensions. We introduce a thin crack at the center of the model with a semi-major axis of length equal to 2 km and a semi-minor axis of length equal to 1 m. To discretize the domain, we use about 45000 Lagrangian elements of quadratic integration order, with size
varying from 150 m at the domain edges and around 1 m at the crack tips. The
dyke is inflated by applying a constant normal pressure on the inner bound-
aries of the fracture. In addition, gravitational and inertial terms are neglected
so that the momentum equation becomes:

\[ \nabla \cdot \sigma = 0 \]  

(4.1)

All three models are based on the linear elastic rheology with elastic mod-
ulus \( K \) equal to 21.3 GPa and \( G \) equal to 15.4 GPa, typical values of a porous
sandstone (David & Zimmerman, 2012). On this basis we modify or add
parameters in function of the tested rheology. For the elastic model with
pressure-dependent moduli, we define \( G \) and \( K \) as a function of pressure (Fig-
ure 4.1). We test three different profiles of \( K \) and \( G \) with varying values in
regions of tensile stresses whereas the maximum values of the elastic moduli

![Pressure-dependent moduli for the non-linear elastic model based on measurement of a Torridonian sandstone (David & Zimmerman, 2012). Three different extrapolation are used in the tensile regime where data are unavailable. a) Shear modulus, and b) bulk modulus as a function of pressure.](image)

Figure 4.1. Pressure-dependent moduli for the non-linear elastic model based on measurement of a Torridonian sandstone (David & Zimmerman, 2012). Three different extrapolation are used in the tensile regime where data are unavailable. a) Shear modulus, and b) bulk modulus as a function of pressure.
Figure 4.2. Temperature dependence of viscosity for dry quartzite host-rock used in the viscoelastic model (Ranalli, 1995).

are kept to $K$ equal to 21.3 GPa and $G$ equal to 15.4 GPa in compressive regions. For the elastoplastic model, we use a Drucker-Prager formulation to define the yield criterion such as:

$$f(\sigma_{ij}) = \sqrt{J_2} - k + \alpha p = 0 \quad (4.2)$$

where $J_2$ is the second invariant of the stress deviator, $\alpha$ is the pressure dependency factor of the yield stress (Paterson & Wong, 2005) and $k$ is a form of cohesion. In this type of rheological model, we test different values of both $k$ and $\alpha$ that we think are appropriate to define crustal or sedimentary rocks. For the viscoelastic model, we use a temperature-dependent viscosity profile that is representative of dry quartzite (Ranalli, 1995) (see Figure 4.2). In order to calculate the heat transport from the dyke into the host-rock, we need to model the material that is within the dyke so that the heat equation can be solved. We thus use constant thermal diffusivity of $\kappa = 1.3 \times 10^{-6}$ m$^2$.s$^{-1}$ for the host-rock and $\kappa = 0.98 \times 10^{-6}$ m$^2$.s$^{-1}$ for the liquid dyke (Clauser & Huenges, 1995). The temperature within the dyke is initially set to $T_0 = 1200$ °C. We run the model until the inner material of the fracture is considered solidified ($T_{\text{solidus}} = 1200$ °C) and that all deformation have ceased.

The elastic theory predicts dykes to be perfectly elliptical in their horizontal cross-section, however observations of dyke thickness indicate more rectangular shapes. We thus define a parameter $m$ in order to describe the shape of the computed dyke, with $m$ defined by the following equation:

$$\left(\frac{x}{a}\right)^{\frac{2}{m}} + \left(\frac{y}{b}\right)^{\frac{2}{m}} = 1 \quad (4.3)$$
where \( a \) and \( b \) are the semi-major and semi-minor axis of the dyke. To summarize, when \( m = 1.0 \) the shape of the dyke is elliptical and \( m \to 0 \) for more rectangular shapes. The three natural dykes that we used to compare our results have a parameter \( m \) that approaches 0.5.

### 4.1.2 Summary

In this paper we test our three rheological models by calculating the required overpressure that will give the best fit to three dyke thickness profiles (A, B and C) measured on the island of Rum (Daniels et al., 2012), and we compared our results with solutions from the linear elastic model (Table 4.1).

**Table 4.1.** Estimated values for required overpressure and shape parameter \( m \) calculated from all the rheological models and for the three tested Rum dykes A, B and C. Values in between parentheses represent the goodness-of-fit between the model and data at the estimated required overpressure.

<table>
<thead>
<tr>
<th>Elastoc</th>
<th>Dyke A</th>
<th>Required Overpressure in MPa, ( m ) parameter, ( (R^2) )</th>
<th>Dyke B</th>
<th>Dyke C</th>
</tr>
</thead>
<tbody>
<tr>
<td>Elastic</td>
<td>466.1, (0.21)</td>
<td>887.1, (0.28)</td>
<td>1617.1, (0.31)</td>
<td></td>
</tr>
<tr>
<td>Elastic with pressure-dependent moduli.</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Wref</td>
<td>418.0.93, (0.30)</td>
<td>817.0.93, (0.36)</td>
<td>1504.0.93, (0.39)</td>
<td></td>
</tr>
<tr>
<td>Wweak</td>
<td>360.0.72, (0.44)</td>
<td>720.0.72, (0.47)</td>
<td>1200.0.72, (0.42)</td>
<td></td>
</tr>
<tr>
<td>Wstrong</td>
<td>441.0.97, (0.25)</td>
<td>852.0.97, (0.31)</td>
<td>1567.0.97, (0.34)</td>
<td></td>
</tr>
<tr>
<td>Plastic, ( \alpha = 0 ).</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>P20</td>
<td>74.0.84, (0.42)</td>
<td>92.0.90, (0.42)</td>
<td>116.0.96, (0.39)</td>
<td></td>
</tr>
<tr>
<td>P100</td>
<td>218.0.68, (0.50)</td>
<td>269.0.74, (0.50)</td>
<td>326.0.80, (0.53)</td>
<td></td>
</tr>
<tr>
<td>P150</td>
<td>283.0.67, (0.50)</td>
<td>354.0.70, (0.52)</td>
<td>429.0.76, (0.54)</td>
<td></td>
</tr>
<tr>
<td>Plastic, depth = 10km.</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>DP0</td>
<td>215.0.62, (0.52)</td>
<td>264.0.66, (0.53)</td>
<td>322.0.72, (0.54)</td>
<td></td>
</tr>
<tr>
<td>DP02</td>
<td>–</td>
<td>–</td>
<td>–</td>
<td></td>
</tr>
<tr>
<td>DP04</td>
<td>440.0.83, (0.32)</td>
<td>764.0.78, (0.41)</td>
<td>1365. –, (0.49)</td>
<td></td>
</tr>
<tr>
<td>DP06</td>
<td>447.0.92, (0.29)</td>
<td>816.0.87, (0.38)</td>
<td>1424. –, (0.45)</td>
<td></td>
</tr>
</tbody>
</table>

We show that the three tested rheological models predict the dyke’s geometry and required overpressure to have a better goodness-of-fit with observational data in comparison to solutions computed from the standard elastic model. All rheological models are interesting because they all enhance deformation but they do it in different ways.

For the elasticity with pressure dependent elastic moduli, we show that a reduction of \( G \) and \( K \) in region of tensile stresses gives significant changes. The model with the greatest rheological weakening Wweak gives a reduction of about 30 percent of the required overpressure in comparison to the linear elastic model (Figure 4.3). In addition, the shape of the resulting dyke is more in accordance with the observational data as indicated by the goodness of fit \( R^2 \) of the calculated thickness profile vs. dyke measurements. Models Wref
and Wstrong also give better fit and lower overpressure than the standard elastic solution but in lower proportion than Wweak (Figure 4.3). The pressure-dependent elastic models mainly show that a reduction of the bulk modulus, which enhance volume changes in region of low pressure, has a minor effect on the opening and shape of the dyke. However, a reduction of the shear modulus, which enhances deformation in regions of high shear stresses, has a big effect on the opening of the dyke and additionally gives dykes with a more rectangular shape by blunting the tips.

As shown in Table 4.1 and Figure 4.4, the elastoplastic rheology has the biggest effect on computed dykes opening and shape. For models with the yield stress independent of pressure ($\alpha = 0$), plastic deformation reduces the required magma overpressure to produced observed dyke thickness by a factor of 5 to 15 for the model with low cohesion (model P20 with $\sigma_y = 20$ MPa). For all three tested models (P20, P100, P150), the calculated overpressures are largely reduced and approach realistic values estimated from other methods. Additionally, plastic models produce dykes with a better fitting shape than solutions computed from the linear elastic model. The best fit is given by the
Figure 4.4. Half-thickness of dyke as function of distance along dyke, both normalized by dyke length. Field measurements for the three dykes on Rum (A, B, and C) are denoted by dots. The continuous curves are the best-fit plastic models without pressure dependence ($\alpha = 0$) and with different yield stress ($\sigma_y = k\sqrt{3}$). Overpressures are most strongly reduced for models with low yield stress, while dyke shape deviates most strongly from the initial ellipse for models with higher yield stress (e.g., shape parameter $m \approx 0.7$ for model P150). We also show results for a model with plane-strain configuration in the third dimension (model P100-2D) instead of the axial symmetry condition of the other models. The plane-strain dyke is much more rectangular ($m \leq 0.6$) because there is less material around the dyke tips relative to total dyke volume which has to be deformed.

For pressure-dependent plasticity models, we keep a constant value for the cohesion ($k = 57.7$ MPa) and vary the pressure dependency factor $\alpha$. For this type of rheology, the overburden increases the cohesion of the host-rock but at the same time, dynamic pressure resulting from the dyke inflation will decrease the material cohesion in the tensile regions surrounding the dyke tips. We show that even a very low value of $\alpha$ drastically changes the outcomes of the model in comparison to a model without pressure dependence on the yield stress. The shape of the dyke and its required overpressure tend to be similar than results from the standard elastic model.
For the viscoelastic rheology, we test two types of system. In the first type, we only test the effect of the host-rock temperature on the evolution of the inflating dyke. The dyke is being inflated at constant overpressure for a fixed length of time $t_{\text{final}} = 10^7$ s, time at which the dyke is considered solidified. For temperature varying from 0°C to 200°C and corresponding to a viscosity of the host-rock varying from $10^{24}$ Pa.s to $10^{18}$ Pa.s, the dyke’s solutions are identical than the linear elastic model. For host-rock viscosity lower than $10^{17}$ Pa.s and corresponding to a background temperature higher than 200°C, we observe significant viscous flow. The uniform low viscosity of the host-rock results in a significant increase of the dyke opening, however it keeps its perfectly elliptical shape. In the second type of viscoelastic models, we take into account the diffusion of the heat contained in the liquid dyke into the host-rock. The dyke is being inflated at constant overpressure for a fixed length of time that is similar than in the first set of model ($t_{\text{final}} = 10^7$ s). The effect of heat diffusion on the host-rock temperature, and hence on the viscous deformation of the dyke’s surroundings, is nearly insignificant for small dykes. The heat transport between the dyke into the surrounding rock only affects a small volume of rock and is mainly ineffective at the dyke tips where we expected enhance deformation. It results that the predicted dyke geometry and overpressure are more or less similar than the solution from the linear elastic model. However, for large dykes, the heat content is enough to significantly decrease the host-rock viscosity at the vicinity of the dyke tips, which causes a change in the dyke shape because this is where stresses are highest.

4.1.3 Conclusions
Our results show significant effects of the three tested rheologies on the calculated dyke geometries and overpressure, each rheology affecting the dyke evolution in different ways:

- Reduced elastic moduli due to the presence of cracks and pores in the host-rock, significantly affect the dyke shape and give a better fit of the overall dyke geometry with observational data. This type of rheology can be applied to the first 2 km of the crust where voids included in the dyke’s surrounding are not yet closed by the lithostatic pressure.

- Elastoplasticity has a large effect on both shape and opening of the growing dyke where lithostatic pressure is negligible (near surface level). At higher depth, the presence of volatile pressure from the magma could balance the effect of the overburden and reduce the frictional resistance of the host-rock. Under those conditions, plasticity could strongly affect the dyke shape and opening independently of depth, temperature and...
Viscoelasticity only affects the dyke surroundings for background temperature higher than 200 °C (for a quartzite host-rock) or if the dyke is large enough to significantly warm up the host-rock. High background temperatures are generally found at deep crustal levels or in region of elevated geotherms, which is typically the case in volcanic areas.

4.2 Paper II: Mechanical energy balance and fracture toughness for dykes in elastoplastic host rock

Paper II addresses the topic of fracture propagation mechanisms applied to magmatic intrusions. In this study, we focus on the concept of fracture toughness and mechanical energy balance of a propagating dyke (mode I fracturing). Most of the previous studies used the linear elastic model to compute the fracture toughness (or fracturing criteria) of mode I cracks (Delaney & Pollard, 1981; Parfitt, 1991; Schultz et al., 2008; Kusumoto & Gudmundsson, 2014), but results are not in accordance with values obtained from lab measurements (Balme et al., 2004; Zhang & Zhao, 2014). The linear elastic model is probably valid at near surface conditions and for low shear stresses (Jaeger et al., 2009), however it does not describe the natural behaviour of rocks at other depths or stress conditions. Indeed, it is well known that at high shear stresses, rocks fail by fracturing in the brittle regime (upper crust), or fail plastically in regions of high temperature (lower crust) (Lawn & Wilshaw, 1975; Ranalli, 1995; Paterson & Wong, 2005). In this study, we then model a dyke propagating in an elastic perfectly-plastic host-rock and we take into account shear fracturing and subsequent frictional slip in the calculation of the fracture toughness. As incremental plasticity is path dependent, we test two geological meaningful end-members cases: 1) A dyke propagating at constant overpressure and 2) a series of dykes inflating pre-existing fractures.

4.2.1 Modelling approach

In this paper, the main objective is to analyse the Griffith energy balance of a propagating dyke and test the effects of the host-rock rheology on the calculation of the different energy components. The Griffith energy balance represents the energy release vs. the energy uptake of a fracture extending by an infinitesimal increment. The equation is generally written as follows:

$$F_{\text{tot}} = \frac{\partial W_b}{\partial a} - \frac{\partial U_e}{\partial a} - \frac{\partial W_{\text{dis}}}{\partial a}$$

(4.4)
Figure 4.5. Model geometry and boundary conditions for all models. A closed dyke with half-length $a$ is placed inside a 2-D domain of host rock with parameters appropriate for a crustal rock (such as granite). Plane strain conditions are used in the third dimension. The domain boundaries far from the dyke are fixed and have negligible effect on the solution. The symmetry boundaries on the bottom and left of the domain are free to slip. A constant pressure is applied normal to the dyke wall.

where $a$ is the half-length of the fracture, $\partial W_B$ is the work input at the boundaries, $U_e$ is the total elastic energy stored in the host-rock and $W_{\text{dis}}$ is the loss of energy due to inelastic deformations. $F_{\text{tot}}$ can also be designated as $G_c$ when the equilibrium state between stability and propagation of the dyke is reached. $G_c$ is linked with the fracture toughness of the rock and can be considered as a material property that represents the energy required by the fracture to propagate through the surrounding rock.

The propagation model consists of a 2-D fracture included in a larger domain of a uniform elastoplastic host-rock in plane strain (see Figure 4.5). To inflate the dyke, we apply a constant pressure condition on the inner boundaries of the nearly closed fracture. The edges of the model are fixed in $x$ and $y$ but the domain is set to be large enough to be sure that stresses have vanished at the boundaries. The material domain is discretized by 11100 triangular elements of varying dimensions, with fine elements at the fracture tips and bigger
elements at the host-rock edges. We use a quasi-static approach for the problem and hence neglect inertial terms and body forces.

In the opposite of the standard elastic model, solutions computed from the incremental plasticity model are path dependent. Therefore, we design two particular paths of propagating fractures that we think are sensible to model the dyke evolution. The first path, namely "Inflation model" describes the inflation of a pre-existing fracture where the second path, "Propagation model" features a dyke that is formed by subsequent fracturing of the surrounding rock.

The yield criterion of the dyke’s host-rock is defined by a Drucker-Prager formulation (Equation 2.2). In a first set of models we make the yield stress independent of pressure so that \( C = \sigma_y \) and we try different values of cohesion. In a second set of models, we introduce a pressure dependency of the plasticity \( \alpha = 0.25 \) and fix the cohesion value to \( C = 15 \) MPa. And for our last test, we take into account the presence of fluid in the damage zone surrounding the crack tips and rewrite the Drucker-Prager formulation for that purpose:

\[
f(\sigma) = \sigma_{\text{mises}} - C - \alpha(p_{\text{ob}} - p_f) - p_{\text{dyn}}
\]  

where \( p_f \) is the fluid pressure, \( p_{\text{ob}} \) is the overburden and \( p_{\text{dyn}} \) the dynamic pressure caused by the dyke inflation and propagation.

The Griffith energy balance of the propagating fracture is calculated for each tested models (see Section 3.5). For simplicity, all of the Griffith energy terms are given as propagation forces that are defined as follow:

\[
F_E = \frac{\partial E}{\partial a}
\]

with \( E \) being one of the energy terms \( U_e, W_b \) or \( W_{\text{dis}} \).

### 4.2.2 Summary

In order to compare the effect of plasticity on the Griffith energy of a propagating dyke, we also run a simple model with a linear elastic host-rock as a reference case (LEFM). Linear elasticity is well understood and known to be path-independent so that it exists one unique model for each final stress conditions. In 2-D, the work done by the magma pressure on the fracture walls, as well as the elastic energy stored in the surrounding rock, are both quadratic functions of the dyke half-length \( a \), thus the corresponding propagation force is linear in \( a \). We show the different propagation forces on Figure 4.6 for a typical crustal host-rock \((G = 35 \text{ GPa and } K = 50 \text{ GPa})\) and a magma over-pressure \( \Delta p = 10 \) MPa. Results show that \( F_b \) is equal to two times \( F_e \) and \( F_{\text{tot}} \), which can be verified analytically for this type of standard elastic rheology (Kusumoto et al., 2013).

In this paragraph, we present the results from the elastic perfectly-plastic rheological models. We observe that for both plastic models (inflation and
propagation models), a process zone (damage or plastic zone) is formed at the dyke tips when the overpressure is of the order of the rock’s yield stress. In addition, the dimensions of that process zone strongly depend on the length and opening of the dyke, but also vary depending on the path taken by the propagating dyke. The inflation model (IF model) has a plastic zone localized at the crack tips whereas the propagation model (PR model) is surrounded by a halo of plastic deformation through the entire length of the dyke (Figure 4.7). In the latter case, the halo is the relict process zones subsequently formed at the tips during the dyke propagation. In Figure 4.8, we show the associated energy balance for both plastic models, with $G = 35$ GPa, $K = 50$ GPa and $\sigma_y = 5$ MPa. Our results are significantly different than the solution from the linear elastic model (see Figure 4.6) because of the energy lost by plastic dissipation in the process zone. We also show that the energy loss due to inelastic dissipation is greater for the PR model than in the IF model and that the amount of the dissipated energy is a function of the size of the process zone shown on Figure 4.7. Plasticity also affects the opening of the fracture and hence the work done by the magma pressure on the fracture walls. As a result, the energy uptake $F_b$ increases for both plastic models. For IF model, the additional boundary work overtakes on the dissipative effects associated with plastic deformation. It results in that plasticity make the fracture less

Figure 4.6. Propagation forces $F$ as functions of half-length $a$ for the linear elastic model with $\Delta p = 10$ MPa, $K = 50$ GPa and $G = 35$ GPa. Dashed lines represent the best linear fit to the model data (stars and dots). $F_e$ and $F_{tot}$ plot on top of each other. All $F$-terms are linear in $a$ because the corresponding energies are quadratic in $a$ due to the two-dimensional model set-up.
Figure 4.7. Plastic strain around a dyke formed by a) propagation (PR model) and b) inflation (IF model) in an elastoplastic host rock with constant yield stress. Result shown is for final increment when half-length \( a = 1 \times 10^4 \) m. Magma overpressure is set to \( \Delta p = 10 \) MPa and yield stress \( \sigma_y = 5 \) MPa. For the propagation model, the dyke is surrounded by a plastic yield zone with width similar to the dyke’s half-length. Much of the plastic zone is the result of the relict dyke tip when the dyke was shorter. The plastic zone may correspond to zone of extensive jointing and brecciation sometimes observed parallel to dykes (Kavanagh & Sparks, 2011; Daniels et al., 2012). For the inflation model, the plastic zone surrounding the dyke tip is similar to that in the PR model, but there is no plastic damage parallel to the central part of the dyke.

stable in comparison to the linear elastic model. In the opposite, the fracture for the PR model is more stable because the energy dissipation overcomes the additional work of the boundary forces.

Results from the pressure-dependent Drucker-Prager PR model (\( \alpha = 0.25 \) and \( C = 15 \) MPa) show that the dynamic pressure (the self-induced pressure state of the inflating crack) has a minor effect on the yield strength. However, we observe that plastic yielding is largely reduced by the effect of the overburden. We show that the model tends to behave like the linear elastic case when the lithostatic pressure is higher than 200 MPa (\( \geq 5 \) km depth). On the other hand, when increasing the fluid pressure (Equation 4.5), the effect of the overburden is cancelled and solutions compare well with the constant yield stress models. However, we do observe small differences that we attribute to the contribution of the dynamic pressure. Indeed, the dynamic pressure reduces the boundary work but also the dissipative plastic loss mainly because regions of positive dynamic pressure are dominant all over the inflating dyke.

4.2.3 Conclusions

In this paper we focused on the effect of an elastoplastic rheology on the dyke propagation energy balance. We show that plastic failure is not limited to a small zone surrounding the crack tip as assumed in the calculation of the
fracture toughness. Instead, inelastic deformation occurs over a large volume, mainly at subsurface level (low overburden) or where fluid pressure is a dominant force in the system. We find that:

- The size of the plastic zone depend on the fracture dimensions and on the ratio between the magma overpressure and the yield stress of the host-rock.

- Plasticity either enhance or suppress dyke propagation depending on the dynamical path taken. PR model has dissipative processes larger than the increase of boundary work associated with plastic deformation so that plasticity causes a reduction of the net force available for the dyke to propagate. IF model has boundary work that dominates over plastic dissipation making dykes less stable against propagation.

- The calculation of fracture toughness assume that inelastic dissipation processes are negligible or constrained to a small zone located at the fracture tips. However, we show that this is not true and that plasticity affects the dyke tips in a larger region. Thus, fracture toughness cannot be used to approximate the effect of large-scale yielding. Instead, it is necessary to explicitly take into account details of large-scale failure.

- This last point can offer an explanation for the long-standing paradox between fracture toughness estimated from the linear elastic model with values obtained from laboratory measurements.

Figure 4.8. Propagation forces $F$ as functions of half-length $a$ for elastoplastic a) PR model and b) IF model with $\Delta p = 10$ MPa, $\sigma_y = 5$ MPa, $K = 50$ GPa and $G = 35$ GPa. Dashed lines represent the best linear fit to the model data (stars, crosses and dots). For IF model, $F_e$ and $F_{\text{tot}}$ plot on top of each other. All $F$-terms are linear in $a$. $F_b$ for the IF model is similar to that of the PR model, but dissipative losses ($F_p$) are reduced by a factor of about 0.5.
4.3 Paper III: Statistical ensemble approach to measure the motion of crystal particles in viscous flow

In paper III, we focus on the rotation of particles embedded in a viscous fluid and we provide the link between their orientation distribution and the dynamics of the flow. It is well-known that solid inclusions are not only advected along the flow, but also rotate around their own axis and sometimes align in the direction of the velocity of the flow. For geological fluids (e.g.: magma), the preferred orientation of a large ensemble of crystals can provide important informations on the flow pattern and its evolution. To this contribution, we use numerical methods to couple the dynamics of crystal rotation (Jeffery, 1922; Willis, 1977; Passchier, 1987; Jiang, 2007; Yamato et al., 2011; Jiang, 2012; Marques et al., 2014) with the Navier-Stokes equation for flows that vary in space and time. To avoid any additional complexities, we preclude interactions between particles and neglect the effect of the particle concentration on the rheology of the flow. Particle orientations are given as a probability density function (PDF) that provides the evolution in time of the preferred (or net) orientation of a particle ensemble at any point of the flow. In our systems, no crystals can be created nor destroyed, thus the probability density function of the particle orientation follows the general concept of conservation. We test our methods against known analytical and numerical solutions for basic flows (March, 1932; Batchelor, 2000; Turcotte & Schubert, 2014), such as: Couette flow, Poisseuille flow, plug flow and corner flow.

4.3.1 Modelling approach

In paper III, we aim to develop the flow theory and the PDF computational methods presented in sections 2.4.1 and 3.6. The objective of that method is to extend the calculation of the net orientation of crystals for heterogeneous flows. We do extensive testing of our solutions against simple systems with known analytical velocity fields. Four of these systems are presented : 1) a 2-D planar Couette flow, 2) a 2-D planar Poisseuille flow, 3) a 2-D planar corner flow (Figure 4.9) and 4) a 3-D Couette flow. In the 2-D models, the particles rotate in the same plane as the flow and around a single axis. The rotation rate in the fixed x-y-coordinate system can thus be given by equation 2.12.

A planar Couette flow is a steady flow that forms in a fluid between two parallel boundaries due to the motion of one of the boundaries relative to the other one (Figure 4.9 a). The resulting velocity field is given by (Turcotte & Schubert, 2014):

\[ v_x = \frac{y v_0}{h} \]  

(4.7)

where \( h \) is the channel thickness and \( v_0 \) the velocity of the moving boundary.

A planar Poisseuille flow is a flow driven by pressure gradients and forms between two fixed plates (Figure 4.9 b). The velocity field is given by (Tur-
Figure 4.9. Sketch of the model setups to illustrate the parameters and boundary conditions. a) Couette flow driven by moving top boundary. The resulting linear velocity profile is shown by arrows. b) Plane Poiseuille flow between two fixed plates driven by a negative pressure gradient \( \frac{dp}{dx} \). Arrows indicate the parabolic velocity profile in \( y \) for constant viscosity \( \mu \). c) Corner flow driven by the bottom boundary which moves to the right with constant velocity \( v_0 \). The left boundary is free-slip, and the remaining boundaries are stress-free. The two-dimensional flow field is shown by arrows.

\[
v_x = \frac{A}{(n+1)} \left( \frac{dp}{dx} \right)^n \left[ \left( \frac{h}{2} \right)^{n+1} - y^{n+1} \right] \quad (4.8)
\]

where \( n \) is equal to 1 for a Poisseuille flow and \( \frac{\partial p}{\partial x} \) is the horizontal gradient of pressure.

In a corner flow, the motion of the fluid is driven by one wall that is moving at a constant velocity while a second wall orthogonal to the first one is defined by free-slip conditions (Figure 4.9 c). The velocity field components for this type of flow are given by (Batchelor, 2000):

\[
v_x = -v_0 \left[ -1 + \frac{2}{\pi} \tan^{-1} \left( \frac{y}{x} \right) + \frac{2}{\pi} \frac{xy}{x^2 + y^2} \right] \quad (4.9a)
\]

\[
v_y = -v_0 \frac{2 y^2}{\pi x^2 + y^2} \quad (4.9b)
\]

For all 2-D flows, we also test our PDF solutions for rectangular crystal shapes. Unfortunately, the right-hand side of equation 2.12 is just valid for elliptical inclusions. To solve this problem, we first build a model of a rectangular particle embedded in a pure shear flow and numerically calculate the
rotation rate in function of the particle angle $\theta$. We then input the results into the right-hand side of equation 2.12.

In the 3-D Couette flow model, we limit our calculation of the crystal rotation to axisymmetric ellipsoidal inclusions. For axisymmetric shapes, two angles are sufficient to describe the orientation of a particle in a three-dimensional space. The principal objective of the 3-D Couette model is to show that our calculation methods of the statistical $PDF$ extends in three-dimension.

For all models, we use a Lagrangian approach, following crystals along their flow paths so that the advection term of the $PDF$ does not have to be taken explicitly. The conservation equation of the $PDF$ is solved numerically using finite element methods and the value of the field $P$ at the initiation of the model is set to $1/\pi$, which describes a random distribution of the crystal orientations.

4.3.2 Summary

In this section we present the $PDF$ of the particles orientation in simple flows and for different crystal shapes and aspect-ratios. Our results are compared to previously published analytical and numerical solutions for similar flows and

![PDF for Couette flow for crystals with high aspect ratio](image)

*Figure 4.10. Numerical solution to (3.16) for $P(\theta)$ for Couette flow and needle-like crystals (using aspect ratio $a/b = 10000$ as an approximation to $a/b \to \infty$) shown by crosses. March’s (1932) analytical solution based on the finite strain ellipsoid is shown for comparison by the solid line. The error in the numerical solution is less than 0.1% for a resolution of 0.01 radians in $\theta$. The solutions are shown for a total strain of $0.5(\varepsilon_1 - \varepsilon_2) = 2.0$.]*
Figure 4.11. PDF of orientations of different crystals in Couette flow. The PDF $P(\theta)$ is given as a function of total strain (which is proportional to time) along the horizontal axis. The scaling of the horizontal axis is such that half of a revolution of an elliptical crystal occurs at a value of unity. a) PDF for elliptical crystal with aspect ratio $a/b = 2$. b) PDF for elliptical crystal with aspect ratio $a/b = 4$. c) PDF for elliptical crystal with aspect ratio $a/b = 10000$, which serves as approximation for $a/b \to \infty$. Unlike the true solution for $a/b \to \infty$, the numerical solution for high but finite $a/b$ eventually exhibits oscillations. d) PDF for rectangular crystal with aspect ratio $a/b = 2$. As the rotation rate for a rectangular crystal is different from that for an elliptical crystal, the completion of the half revolution does not occur exactly at $(\epsilon_1 - \epsilon_2)ab = \pi(a^2 + b^2)$, but about 10% earlier.
similar particle geometries (Jeffery, 1922; March, 1932; Willis, 1977; Passchier, 1987; Jiang, 2007; Marques et al., 2014).

For the Couette flow model, March (1932) provided an analytical solution that describes the PDF evolution of a needle-like (infinite aspect-ratio) ellipsoidal crystal. The numerical PDF solution for a crystal of aspect-ratio tending to infinity \(a/b = 10000\) is compared with the analytical solution provided by March (1932). Results are shown on Figure 4.10. The overall fit is perfect. For a Couette flow, all crystals rotate toward \(\theta = 0\) regardless of their initial position because their stable orientation is aligned in the direction of the flow (Figure 4.11 c).

For crystals with finite aspect-ratio (Figure 4.11 a and b), the evolution of the PDF is very similar than for a needle-like crystal. In fact, it is only the rotation due to pure shear which is reduced by a factor of \(\frac{a^2 + b^2}{a^2 - b^2}\) (Equation 2.12). This small difference in the rotation rate has a major effect on the behavior of the crystal dynamics and on the evolution of the PDF. For
this type of aspect-ratio, the behaviour of the crystal is largely dominated by the solid body rotation component, even when the crystal is oriented in the direction of the flow ($\theta = 0$). At that orientation, the crystal rotates more slowly and never reaches a stable orientation but instead keeps rotating perpetually in a clockwise direction. For a particle of a given aspect-ratio, a complete rotation always takes the same total of strain regardless of the crystal’s initial orientation. Figure 4.11 shows the evolution of the PDF in function of ratio $\varepsilon_{1/2} = (a^2 + b^2) \pi/2ab$. Within this frame, a full particle revolution occurs from $\varepsilon_{1/2} = 0$ to $\varepsilon_{1/2} = 1$. Starting with a random orientation at $\varepsilon_{1/2} = 0$, a broad peak of low magnitude starts to form around $\theta = \pi/2$. The peak gradually grows and shifts until reaching a maximum at $\theta = 0$. The peak then continues to migrate but the magnitude decreases and the PDF reaches its initial configuration at $\varepsilon_{1/2} = 1$. For the same aspect-ratio, the PDF evolution for a particle of rectangular shape (Figure 4.11 d) is really similar than solutions from the ellipsoidal shape. This result is in accordance with other studies (Willis, 1977; Schmid, 2005; Fries et al., 2017), which show that the crystal’s shape has a minor influence on the rotation dynamics. We do however observe some minor effects on the recursion time of the particle revolution and on the magnitude of the PDF peak.

For the Poisseuille flow model, we show in Figure 4.12 the net orientation of ellipsoidal particles as tick marks. Additionally we define a degree of orientation of the PDF as:

$$R = \left[ \left( \int_0^\pi P \cos(2\theta) \, d\theta \right)^2 + \left( \int_0^\pi P \sin(2\theta) \, d\theta \right)^2 \right]^{1/2}$$  \hspace{1cm} (4.10)

When $R$ is zero, the PDF follows a uniform distribution and when $R$ is equal to unity, the PDF is an appropriately normalized Dirac delta function. According to the boundary conditions that we imposed, the PDF has a zero degree of orientation at the inflow (left-wall, see Figure 4.9 c). Along the central line of the channel, the strain rate is 0 and thus the rotation rate defined by equation 2.12 is also 0. Along that location, the PDF remains uniform, independently of the residence time of the particles. However, the strain rate and hence the rotation rate have their magnitude being maximal at the edges of the flow. Consequently the period of the particle revolution as a function of $x$ decreases from the center of the channel toward the edges.

For the 2-D corner flow model, the PDF evolution and particle orientations along different stream lines are summarized on Figure 4.13. Over the entire domain, the orientation of the PDF peak exhibits only minor changes. We do observe changes in the degree of orientation nearby the bottom boundary, where the velocity field and thus the strain rate are maximum. The complete PDF along stream lines 1 and 9 are shown on Figure 4.14 a and b. The dominant orientation of particles at the vicinity of the corner point is about 40° along line 1 and about 25° along line 9. Along the moving bottom wall, parti-
Figure 4.13. Representation of PDF of crystal orientations for elliptical crystals ($a/b = 2$) for corner flow as a function of position. Tickmarks indicate orientation that corresponds to the local peak of the PDF. Shading shows the degree of orientation $R$. Near the origin, the flow field changes rapidly as a function of position, leading to fairly abrupt local changes in the PDF.

Particles following stream line 1 get progressively reoriented horizontally. At that location the flow becomes nearly identical to a Couette flow and thus the dynamics of the particles progressively tend to look like the solution from the 2-D Couette flow model.

The results from the 3-D Couette flow are not shown here because they simply repeat what we observe in the 2-D Couette flow model. However, it shows that our computational methods also work for the 3-D rotation evolution of an elongated particle.
4.3.3 Conclusions

The existing methods of crystal rotation calculation for homogeneous flows (Jeffery, 1922; Jiang, 2007; Marques et al., 2014) are extended in this study to flows that vary in space and time. One other major feature of this work is the integration of a probability density function to describe the rotation dynamics of suspended solid particles. Throughout paper III, we show that:

- Our results of the simple models (Couette flow and Poisseuille flow) compare almost perfectly with previously published analytical and numerical solutions. We can then be fairly confident in the veracity of our methods and hence on the calculation of a PDF for particles suspended in more complicated flows (e.g. corner flow).

- The calculation of the PDF can be extended to any kind of particle shape on the condition that a rotation rate profile as a function of orientation can be provided.
• Coupling between the PDF evolution of crystal orientation with the Navier-Stokes equation of fluid should enable the analysis of crystal dynamics in more complex systems (magmatic systems).

4.4 Paper IV: Crystal rotations and alignment in spatially varying magma flows: Two-dimensional examples of common subvolcanic flow geometries

In geology, several techniques of observation can provide indications on the relict magma flow, such as AMS analysis (Tauxe et al., 1998; Canon-Tapia & Chavez-Alvarez, 2004; Cañón Tapia, 2004; Palmer et al., 2007; Eriksson et al., 2011) or direct observations of crystal alignment in solidified magmatic complexes (Clemens, 2003; Pons et al., 2006; Vernon & Paterson, 2006). However, the configuration of these flow indicators only relates to the last increment of strain before solidification of the complex. In paper IV, we aim to provide the link between flow indicators such as elongated particles with the dynamics of magmatic reservoirs. To do so, we use the computational and statistical methods developed in paper III and apply them to common subvolcanic flows. We present five typical examples: an inflating or deflating magma reservoir, a magma entering or exiting a planar channel, and a thermal convection flow in a magmatic reservoir.

4.4.1 Modelling approach

In our models, all crystals rotate along a single axis with \( \theta \) describing the rotation angle between the horizontal direction and the major axis of the elongated particle. The rotation rate of the crystal suspended in the flow is given by equation 2.12. The net orientation of the particle ensemble is given as a probability density function \( P(x, y, \theta, t) \) that is conservative in time (Equation 3.16). We use numerical methods to solve the Navier-Stokes equation of the Fluid and thermal properties of the material for the convection model, with \( \mu \) the viscosity, \( \rho_0 \) the reference density, \( \alpha \) the volumetric expansion coefficient, \( k \) the thermal conductivity and \( c_p \) the specific heat at constant pressure.

<table>
<thead>
<tr>
<th>Parameters</th>
<th>Values</th>
<th>Units</th>
</tr>
</thead>
<tbody>
<tr>
<td>( \mu )</td>
<td>7 \times 10^6</td>
<td>Pa.s</td>
</tr>
<tr>
<td>( \rho_0 )</td>
<td>2800</td>
<td>kg.m(^{-3})</td>
</tr>
<tr>
<td>( \alpha )</td>
<td>3 \times 10^{-5}</td>
<td>1.K(^{-1})</td>
</tr>
<tr>
<td>( k )</td>
<td>2.25</td>
<td>W.m(^{-1}).K(^{-1})</td>
</tr>
<tr>
<td>( C_p )</td>
<td>750</td>
<td>m(^2).s(^{-2}).K(^{-1})</td>
</tr>
<tr>
<td>( \Delta T )</td>
<td>400</td>
<td>°K</td>
</tr>
</tbody>
</table>
fluid (magma) and couple the velocity field with the evolution in time and space of $P$.

The first set of model describes the transition between a magmatic intrusion and a larger reservoir. The model domain is defined by a square of dimension $10 \times 10$ m, representing the reservoir and connected in the middle of its right edge to a rectangle of dimensions $5 \times 1$ m, representing the conduit. In the first transition model, the flow enters the system at the right edge of the conduit at a fixed velocity of $10 \text{m.s}^{-1}$ and leaves at the left edge of the reservoir. In an opposite model, the flow enters the system from the left side of the reservoir at a fixed velocity of $1 \text{m.s}^{-1}$ and leaves at the right side of the conduit. No-slip boundary conditions are applied on every walls except for the flow inlet and outlet. Before computation, the field $P$ is set to be constant over the domain with $P = 1/\pi$, which describes a random distribution of the particle orientation. We apply the same conditions at the flow inlet and outlet.

The second model describes the inflation and deflation of a magma chamber. For the inflating chamber, the model domain is defined by a sphere of radius $r$ equal to 1 m, that is inflating in function of time. After a running time of $t_{\text{final}}$ equal to 1 s, the radius of the sphere has effectively doubled, thus $r_{\text{final}}$ is equal to 2 m. To compensate the inflation of the chamber, we add a small inlet at the bottom of the model where the fluid is injected at a a constant surface flow rate of $2\pi \text{m}^2\text{s}^{-1}$. For the deflating chamber, the radius of the sphere decreases from 2 m to 1 m and the outlet is located at bottom of the sphere. Before computation, the field $P$ is set to be constant over the domain with $P = 1/\pi$. We apply the same conditions for the flow inlet and outlet.

Our final model is a large rectangular box that is $100 \times 50$ m in dimension and containing convective magma. All walls have free slip conditions and the top and bottom edges have constant temperature conditions with $T_{\text{top}} = 1475^\circ \text{K}$ and $T_{\text{bottom}} = 1075^\circ \text{K}$. Additionally, the side walls are thermally isolated so that $\partial T / \partial x = 0$. The convection is driven by the contrast of density between the light and hot material and the heavier and cold material. The density function $\rho(T)$ is given by equation 3.8 and with $\alpha$ the expansion factor equal to $3 \times 10^{-5} \text{K}^{-1}$. The Rayleigh number of the flow is around 2000 which results in the formation of steady convection cells. Before computation, the field $P$ is set to be constant over the domain with $P = 1/\pi$.

For all our models, we show the vorticity number at each location of the flow, which defines the ratio of the solid-body rotation rate to the pure shear stretching rate. The vorticity number is computed as follows:

$$ W_k = \frac{\sqrt{2} \Omega}{(\dot{\varepsilon}_1 + \dot{\varepsilon}_3 + \dot{\varepsilon}_3)^{1/2}} \quad (4.11) $$

where $\Omega$ is the magnitude of the angular velocity vector. For high vorticity number, the solid body rotation is high and works against the alignment caused
by pure shear because the vorticity of the flow rotates the crystal out of the pure shear field.

4.4.2 Summary

The objective of this paper is to show preferred orientations of elongated particles suspended in magma flow and in dynamical systems that are representative of magma dynamics in the volcanic plumbing system.

The first set of models describe a magma exiting or entering a planner channel. The velocity field, vorticity number and particle orientation for both mod-

Figure 4.15. Results for the models of the transition between a channel and a reservoir. Left-hand panels are for flow exiting from the channel into the reservoir, right-hand panels are for the reverse flow. a) and d) velocity magnitude (shading) and direction (arrows) of the fluid flow. b) and e) vorticity number (shading) and orientation of $\dot{\varepsilon}_1$ (tick marks). c) and f) degree of orientation of the PDF (shading) and most likely orientation (peak of PDF) of particles with aspect ratio $a/b = 2$ (tick marks). In the conduit-to-reservoir model, particles mostly align perpendicular to the flow direction, while in the tank-to-conduit model, particles align in the direction of flow.
els are shown on Figure 4.15. In the first model (see Figure 4.15 a), the material flows from a thin conduit into a large reservoir. The resulting crystal orientations, summarized in Figure 4.15 c, show a complex behaviour. In the

Figure 4.16. Results for the models of inflation and deflation of a magmatic reservoir. In the inflation and deflation model, the fluid enters or exits the system from the inlet and outlet located at the bottom of the reservoir. a) and d) velocity magnitude (shading) and direction (arrows) of the fluid flow. b) and e) vorticity number (shading) and orientation of $\dot{\varepsilon}$ (tick marks). c) and f) degree of orientation of the PDF (shading) and most likely orientation (peak of PDF) of particles with aspect ratio $a/b = 2$ (tick marks). In the inflation model, particles mostly align perpendicular to the flow direction, while in the deflation model, particles align in the direction of flow.
conduit, a Poisseuille flow develops and particles orient themselves parallel to the direction of flow. Past the conduit, a strong crystal alignment develops in the middle of the reservoir due to pure-flow stretching. At that location, crystals get reoriented perpendicular to the flow direction but parallel to $\dot{\varepsilon}_1$. Near the reservoir walls, the flow is well approximated by a Couette flow and the preferred orientation of crystals is approximately parallel to the walls. For the reverse flow field (see Figure 4.15 d), crystal orientations are summarized on Figure 4.15 f. Essentially, crystals get oriented in the direction of the flow, pointing toward the entrance of the thin channel. The results of those two transition models are in accordance with conclusions of analogue modelling studies (Závada et al., 2009; Trebbin et al., 2013) where a similar behaviour of particle orientations is observed.

![Figure 4.17](image)

*Figure 4.17. Results for the thermal convection flow model with Rayleigh number equal to 2000. a) velocity magnitude (shading) and direction (arrows) of the fluid flow. b) vorticity number (shading) and orientation of $\dot{\varepsilon}_1$ (tick marks). c) degree of orientation of the PDF (shading) and most likely orientation (peak of PDF) of particles with aspect ratio $a/b = 2$ (tick marks). Thermal convection causes crystal alignment parallel to the walls where the flow due to convection cells impinges on the boundary, and where flow is parallel to the boundaries. Crystal alignment is normal to the walls where the flow turns away from the boundary.*
For the inflating and deflating magma chamber (or reservoir), the evolution of the PDF is mostly similar than in the two previous transition models as shown on Figure 4.16. For the inflating chamber, the flow field is dominated by pure-shear stretching parallel to the reservoir walls. However, the flow pattern is largely perturbed by the flow inlet causing $\dot{\varepsilon}_1$ to be inclined by $45^\circ$ relative to the walls. In the inflating model, a strong crystal alignment pattern develops parallel to the wall at the edge of the reservoir, and perpendicular to the flow near the middle. We observe the opposite behaviour for the deflating chamber model where particles mostly aligned in the direction of flow, pointing toward the outlet section located at the bottom of the model. Nearby the edges of the deflating chamber, particles are oriented perpendicular to the walls.

For our last model, the crystal alignment pattern in the convection cells are slightly more complex. We show that in the up-wellings and down-wellings of the convective cells, particles are mostly aligned both in the direction of flow and in the direction of $\dot{\varepsilon}_1$ (see Figures 4.17 b and c). Along the bottom and top boundaries, the flow is essentially a Couette flow and $\dot{\varepsilon}_1$ is oriented parallel to the walls. At these location, a strong alignment pattern forms parallel to the wall and in the direction of the flow. In the middle of the convective cells, the suspended particles seem to follow an organised pattern with $\theta$ being around $20 - 30^\circ$. In these locations, the rotation due to solid body rotation component of the flow is high (shown by the vorticity number on Figure 4.17b), which will de-organised the alignment pattern of particles due to pure shear. This is confirmed by the low degree of orientation located at the center of the convective cells.

4.4.3 Conclusions

In paper IV, we present numerical results for the magma velocity field and for the PDF of crystal orientations in common subvolcanic flow geometries.

- For magma exiting a dyke and entering a larger reservoir, we find that, away from the walls, elongate crystals preferentially align in the local direction of $\varepsilon_1$, which is perpendicular to the flow direction at the dyke-reservoir transition. For the reverse flow of magma entering a dyke, both $\varepsilon_1$ and the crystals align with the direction of the flow. This observation is in good agreement with results from analogue models.

- In an inflating magma reservoir with uniform stretching of the bounding walls, crystals become aligned parallel to the walls throughout the domain except for the immediate vicinity of the inflow into the reservoir. For the reverse model of a deflating reservoir, the corresponding crystal orientations are radial and hence perpendicular to the walls.
• Thermal convection causes crystal alignment parallel to the walls where the flow due to convection cells impinges on the boundary, and where flow is parallel to the boundaries. Crystal alignment is normal to the walls where the flow turns away from the boundary.

• Our method solves the forward problem of finding preferred crystal orientations from the velocity field, and hence from the basic underlying dynamics. For typical applications, it is the inverse problem that needs to be solved, which consists of inferring the flow and its dynamics from observations of crystal orientations. An inherent difficulty of the inverse problem is nonuniqueness when isolated subdomains are considered. For example, boundary-parallel orientations may indicate boundary-parallel shear flow, or they may indicate pure shear flow impinging on the wall. For such cases, it is necessary to find a globally consistent flow field. On the other hand, crystal orientations normal to the boundary are probably good indicators of thermal convection, because the competing candidate, namely a local contraction of the boundary such as in a deflating reservoir, is physically unlikely to occur.
5. Conclusions

In this thesis, we have presented numerical methods and tools that aid in our understanding of the volcanic plumbing system.

First, the numerical models provide new insights into the formation and propagation of pressurized fractures such as magmatic intrusions. We aimed to show that the model of linear elasticity does not properly describe the behaviour of rocks in regions of high shear stresses, or in regions of elevated temperatures. Instead, other mechanisms of deformation have to be considered such as plastic or ductile flow of the rock. We show that the host-rock rheology has a major influence on the thickness, shape, pressure and propagation criteria of a growing sheet like-intrusion. Results from all the tested rheological models, namely pressure-dependent elastic, elastoplastic and viscoelastic, are highly different than solutions from the linear elastic model. Instead, solutions are more in accordance with natural observations. Among all the mentioned models, the elastoplastic model has the largest effect on the shape, opening, magma pressure and fracture toughness calculation of a growing dyke. However, the effects of plasticity are mostly constrain to the uppermost 1 – 2 km of the Earth’s crust. At deeper levels, the lithostatic pressure is dominant and cancel out the effect of plasticity. Elevated pore pressure due to exsolving volatiles from the magma would facilitate the brecciation of the rock at the intrusion tips and decreases the frictional resistance to slip on the new surfaces. If the pore pressure is high enough to cancel the effect of the overburden, the plastic yield can be considered as independent of pressure and thus independent of depth. We also show that the model of viscoelasticity has the potential to greatly affects the evolution of the dyke. However, the effects of ductile flow on the shape and opening of the dyke are limited to regions of very high temperature, or for dykes of large volume in which the heat content is large enough to significantly affects the rheology of the surrounding rock.

Calculation of fracture toughness is based on the simple assumptions that the host-rock rheology of the magmatic intrusion (or mode I fracture in general) is linearly elastic and that plastic yielding is limited to a small process zone located at the tips. We show from our elastoplastic models of dyke propagation and inflation that this assumption is wrong and that the plastic zone affects a large area along the dyke length and/or at the tips, specially if the magma overpressure is of the order of the host-rock yield stress. Dissipation of energy results from large scale failure of the intrusion’s host-rock and cannot be neglected or constrained to a small region localized at the intrusion tips. Dimensions of the process zone are strongly dependant of several parameters:
the ratio between magma overpressure and the yield criterion of the host-rock and the intrusion length. The elastoplastic model additionally shows that the Griffith energy balance, and the fracture toughness, of a propagating dyke is strongly dependent on its dynamical path. For a dyke propagating at constant driving pressure, plastic deformation tends to impede dyke growth, whereas for a dyke inflating in a pre-existing fracture, plasticity enhances dyke growth. For the propagation model, the energy dissipated in the large damage zone can explain the mismatch between fracture toughness calculation from the linear elastic model with fracture toughness measurements from laboratory experiments.

In the second part of the thesis, the numerical method of crystal orientation calculation couple with the numerical computation of the Navier-Stokes equation, aim to provide the link between active flows and observations of crystal alignment in solidified magmatic systems. A statistical approach is used to describe the orientation of a large particle ensemble. This way, we can estimate the net or mean orientation of crystals at any point in space and time of a viscous flow. This approach is particularly useful for geological flow in which the bulk orientation of crystals can provide useful informations on the flow evolution. In addition, the coupling between crystal orientation and the Navier-Stokes equation for flows enables analysis of crystal alignment in any type of complex system such as non-Newtonian flows or flows with a complex structure and complex boundary conditions. The method can also be extended to any type of particle shape in condition that the rotation rate component due to pure shear flow is provided. Results obtained from our crystal analysis for magma flow systems generally compare well with field observations, AMS, magmatic fabrics or analogue models. Our methods can thus provide a way to test a given hypothesis of flow (or flow dynamics) for given crystal orientation observations.
tionsdynamiken till Navier-Stokes ekvation i storskaliga flöden. Vi introduc-
erar även en differentialekvation för utvecklingen av sannolikhetsdensitets-
funktionen (PDF). Efter omfattande testning applicerar vi den nya metoden
 till ett antal enkla flödesexempel för att öka förståelsen för hur realistiska
flödesmönster påverkar kristallriktningen.

I artikel I modelleras uppumpningen av en tvådimensionell plattliknande
intrusion inbäddad i en kontinuerlig berggrund. I början av beräkningen repre-
senteras intrusionen av en stängd spricka som sedan öppnas av ett tryckvillkor
 riktat utåt på sprickans inre gräns. Tjockleken på sprickans profil beror då
på tryckvillkoret och omgivande berggrunds reologi (deformation- och flöde-
segskaper av ett material under applicerat tryck), därför testas tre olika re-
ologiska modeller vilka är baserade på den linjära elastiska modellen, men
tillåter för en mer realistisk reologisk modell och kartlägger effekten på sprick-
ans beräknade tjockleks profil. I modell I är den elastiska modulen kring spri-
ckan tryckberoende för att ta hänsyn till bildning och stängning av mikro-
sprickor, hålrum och porer i regionen av drag- och kompressionsspänning. I
den elastoplastiska modellen tas hänsyn till brott genom sprickbildning och
friktionsglidning i regionen av hög skjuvsspänning. Till sist, i den viskoel-
astiska modellen, testas effekten av plastiskt flöde i berggrunden genom kryp-
mekanismer i regioner med hög temperatur. Våra resultat visar på signifikan-
ta effekter av de tre testade reologiska modellerna på de beräknade gångarnas
geometri och tryck. Trycket som krävs för den elastoplastiska modellen att passa
data är för en given spricktjockleks profil är 70 – 90 % lägre än i lösningen för
den linjärelastiska modellen.

I artikel II räknar vi ut energibalansen av en propagerande spricka inbädd-
dad i en elastoplastisk berggund och jämför resultaten med den linjärelastiska
lösningen. Våra modelleringstekniker är väldigt lika de i artikel I bortsett
från att sprickorna inte bara pumpas upp utan även propagerar från extrem-
iteterna. I denna studie testas två typer av sprickpropagering. I den första
sker propageringen genom en kontinuerlig uppsprickning av berget (propaga-
tion model) och i den andra modellen utvecklas sprickan genom successiva
episoder av uppumpning och inträngande av magman i ett redan befintligt
svaghetsplan (inflation model). Våra resultat visar att plastisk deformation
försvårar tillväxten av gångar när det sker genom propageringsmodellen, me-
dan den underlättar i uppumpningsmodellen. Vidare visar plasticiteten effekt
på uträkningen av apparent sprickhårdhet för vår propageringsmodell värden
som är 10 – 100 lägre än för den linjärelastiska modellen, men av liknande
magnitud som laboratoriumävda värden.

I artikel III och IV vill vi kartlägga den föredragna orienteringen av långs-
sträckta kristaller i ett visköst flöde. Syftet med artikel III är att utveckla
en beräkningsmetod som beräknar effekten av flödesrörelsen på rotationen av
kristallerna. Det lokala flödesfältet (eller hastighetsfältet) kan sålunda de-
las in i enskilda komponenter vilka har en distinkt effekt på rotationen av
kristallerna. Inklusionernas riktning bestäms av en statistisk sannolikhets-
desitetsfunktion som lokalt indikerar riktningen av den stora kristallansamlingens. För att testa våra metoder beräknar vi den föredragna orienteringen av långsträckta partiklar längs en strömlinje av ett couetteflöde, poisseuilleflöde och hornflöde. Vi jämför sedan våra resultat mot kända analytiska lösningar och visar att våra metoder ger resultat som passar perfekt med dessa lösningar. I artikel IV tillämpade vi således våra beräkningsmetoder för tvådimensionella flöden som hänför sig till ett mer realistiskt system av magmacirkulation: en uppbäst magmakammare, en magma som strömmar från en stor reservoar till en platliknande intrusion och viceversa och ett konvektivt flöde i en stor magmatisk reservoar.
7. Acknowledgements

And here we are, five years later. Five years of a long and difficult process that pushed me to my limits and sometimes beyond (specially the last three months). But what an amazing and fruitful journey it was! It wasn’t easy at first though, leaving the warmth and comfort of my friends and family behind, leaving the warmth (dot), starting a new nest from scratch one more time, in a town where finding your own apartment is as easy as staying sober at a TGIF. But little by little I managed to build my own circle and I guess i wasn’t too bad at it. So many people entered in my life and left me with unforgettable souvenirs and memories. And this section is dedicated to all of you, the people who made this adventure possible and unforgettable for me.

First, of course, I would like to thanks my supervisor Chris Hieronymus, who offered me the possibility to do this thesis. We didn’t really follow the original plan of study but it really does not matter as I learnt a lot about volcanoes, dykes, fracturing, physics, modelling, all mostly thanks to him. His knowledge was really precious during those five years and he managed to lead me from mountains to fracture and fluid mechanics. We had a very different background at the beginning and it wasn’t always easy to understand each other (also mostly because of my French accent), but i think we managed and i am really proud of the work we accomplished together. I now hope that I can learn and master all of his lessons and hopefully i can be as a good scientist as him later. I would also like to thank my second supervisor Chris Juhlin who was mostly the face of authority in my PhD (he is the prefect after all), pushing and confronting me when things weren’t going well but always staying fair, helpful and supportive. Geocentrum is really lucky to have someone like him at the head of the department.

I would also like to say thank you to all the other researchers with who i shared the passion of rocks. Thank you Steffi, Hemin, Bjarne, David, Alireza, Peter, Jarek, Iwona, Tobias, Erika and all the other people from the Mountain and Volcano working groups. A big thanks to all the people at the administration who made my life much easier at university. A special thanks to Fatima who was amazing (and very patient) with me during all those years. Her kindness is a real help for us, the little PhD students, and we are all lucky to have her here.

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