GEOPHYSICAL AND GEOCHEMICAL ANALYSES OF
FLOW AND DEFORMATION IN FRACTURED ROCK

A thesis summary

by

Joshua Taron
The six chapters of this thesis correspond with a series of six primary publications. By order of chapter appearance, these papers are:

Taron, J., Elsworth, D., and K.-B. Min (2009)

*International Journal of Rock Mechanics and Mining Sciences (vol. 46)*

Numerical simulation of thermal-hydrologic-mechanical-chemical processes in deformable, fractured porous media

Taron, J. and D. Elsworth (2009)

*International Journal of Rock Mechanics and Mining Sciences (vol. 46)*

Thermal-hydrologic-mechanical-chemical processes in the evolution of engineered geothermal reservoirs

Taron, J. and D. Elsworth (2009)

*Journal of Geophysical Research (vol. 115)*

Constraints on compaction rate and equilibrium in the pressure solution creep of quartz aggregates and fractures: Controls of aqueous concentration

Taron, J. and D. Elsworth (2009)

*International Journal of Rock Mechanics and Mining Sciences (vol. 47)*

Coupled mechanical and chemical processes in engineered geothermal reservoirs with dynamic permeability

Taron, J., D. Elsworth, G. Thompson, and B. Voight (2007)

*Journal of Volcanology and Geothermal Research (vol. 160)*

Mechanisms for rainfall-concurrent lava dome collapses at Soufrière Hills Volcano, 2000-2002


*Science (vol. 322)*

Implications of magma transfer between multiple reservoirs on eruption cycling
Abstract

Under geophysical and geochemical forcing whole and fractured rock exhibit dynamic characteristics of hydraulic transport and mechanical deformation. Changes to permeability, porosity, and compressibility can be rapid and significant, with short- and long-term variability of intrinsic rock and fracture properties linked intricately to the applied forces: temperature, fluid pressure, mechanical stress, and chemical potential. The magnitude and interaction of these applied forces and controlling parameters govern fluid circulation in geothermal reservoirs, transport and trapping mechanisms in the sequestration of carbon dioxide, saturation state surrounding high temperature radioactive waste, fluid circulation and recovery in petroleum reservoirs, pressure dissipation rate within active fault zones, and the failure potential of volcanic domes, to name a few.

To a far greater extent than many anthropogenic materials, rocks are defined by anisotropic and discontinuous material properties. And, as in any scientific analysis, complex mechanisms are often best approximated by determining the rate-limiting step, or the variable that defines most strongly an observable process. For fluid flow and deformation within earth materials, it is often the discontinuous features that define behavior: fractures.

The following is a study of fluid flow and deformation in fractured rock, with particular emphasis on environments under thermal and chemical stress. Because of their significance, fractures are treated in the greatest detail, with constitutive modeling at pore and reservoir scale, and their impact explored with reservoir scale numerical simulation. Part I of this thesis (Chapters I-IV) explores the behavior of engineered systems pushed far from equilibrium and highlights feedbacks between stress and chemistry on the evolution of the mechanical and transport properties of rocks; these observations and analyses are focused on the behavior of geothermal reservoirs. Part II (Chapters V-VI) examines the response to natural forcing and follows the complex interactions that shape processes in volcanic environments.

Part I: Engineered Environments

Chapter I introduces a method to couple the thermal (T), hydrologic (H), and chemical precipitation/dissolution (C) capabilities of TOUGHREACT with the mechanical (M) framework of FLAC\textsuperscript{3D} to examine THMC processes in deformable, fractured porous media. The combined influence of stress-driven asperity dissolution, thermal-hydro-mechanical asperity compaction/dilation, and mineral precipitation/dissolution alter the permeability of fractures during thermal, hydraulic, and chemical stimulation. Fracture and matrix are mechanically linked through linear, dual-porosity poroelasticity. Stress-dissolution effects are driven by augmented effective stresses incrementally defined at steady state with feedbacks to the transport system as a mass source, and to the mechanical system as an equivalent
chemical strain. Porosity, permeability, stiffness, and chemical composition may be spatially heterogeneous and evolve with local temperature, effective stress and chemical potential. Changes in total stress generate undrained fluid pressure increments which are passed from the mechanical analysis to the transport logic with a correction to enforce conservation of fluid mass. Analytical comparisons confirm the capability of the model to represent the rapid, undrained response of the fluid-mechanical system to mechanical loading. A full thermal loading/unloading cycle is explored in a constrained fractured mass to follow irreversible alteration in in-situ stress and permeability resulting from both mechanical and chemical effects.

Building upon the model presented in Chapter I, Chapter II examines some of the dominant behaviors and permeability-altering mechanisms that may operate in naturally fractured media. A prototypical enhanced geothermal system (EGS) is examined for the relative, temporal arrival of hydro-mechanical vs. thermo-mechanical vs. chemical changes in fluid transmission as cold (70°C) water is injected at geochemical disequilibrium within a heated reservoir (275°C). For an injection-withdrawal doublet separated by ~670m, the results demonstrate the strong influence of mechanical effects in the short term (several days), the influence of thermal effects in the intermediate term (<1 month at injection), and the prolonged and long-term (>1 year) influence of chemical effects, especially close to injection. In most of the reservoir, cooling enhances permeability and increases fluid circulation under pressure-drive. Thermomechanical driven permeability enhancement is observed in front of the advancing thermal sweep, counteracted by the re-precipitation of minerals previously dissolved into the cool injection water. The importance of the coupling between reactive transport and geomechanics is illustrated. Mineral behaviors alter fluid flow paths and, in so doing, change the characteristics of thermo-hydro-mechanical aperture changes, and vice versa. Each incurs changes in the system that fundamentally alter the evolutionary paths of reaction and chemical/mechanical deformation in a manner that mandates the accommodation of process couplings for the full THMC suite of interactions.

Chapters III and IV evolve from a need to represent mechanical strain, chemical-mechanical creep, and shear dilation as innately hysteretic and interlinked processes. To do so requires the reanalysis and development of a micromechanical constitutive theory of pressure solution in quartz materials. This is the purpose of Chapter III. A relationship is developed to examine dissolution precipitation creep in crustal rocks with implicit coupling of the dissolution-diffusion-precipitation system without requiring the iterative solution of a linear equation system. Implicit control is maintained over aqueous silica concentrations within hydrated solid contacts and in open pore space. For arbitrary conditions of temperature, pressure, and mechanical stress the simple equation system conforms to a polynomial solution for aqueous concentrations set within a small iterative compaction scheme. Equilibrium (long-
term) pressure solution compaction, previously ill-constrained, is explored with two alternate methods: 1) A modified form of critical stress and 2) Rate controlled growth of diffusion limiting cement at the periphery of solid contacts. Predictions are compared to previous experimental results that allow compaction equilibrium to be achieved. Only the modified critical stress is capable of reproducing these results. In this case, the agreement is strong across a range of conditions (400-500°C, 20-150 MPa, and 3-60 μm mean particle diameter) and without parameter adjustment. Predictions are also compared to concentration independent simplifications at general conditions of 350°C and 100 MPa. Compared to the implicit coupling, these methods represent the mean behavior; slightly underestimating rates in dissolution control, and slightly overestimating in diffusion control. Both regimes may be important at upper crustal conditions. The solution is extended for open and closed systems and is applicable to granular media and fractures, differing only in the method defining evolving contact geometry.

Chapter IV presents a model to represent mechanical strain, stress-enhanced dissolution, and shear dilation as innately hysteretic and interlinked processes in rough contacting fractures. This model is incorporated into the numerical simulator of Chapters I and II. A candidate engineered geothermal reservoir system (EGS) is targeted. The new mechanistic model is capable of distinguishing differences between the evolution of fluid transmission characteristics of 1) small scale, closely-spaced fractures and 2) large scale, more widely spaced fractures and their impact on permeability evolution and thermal drawdown within the reservoir. The presence of longer and more widely-spaced fractures within a reservoir is shown to be potentially significant and capable of causing both hydraulic and thermal short circuiting. Such a process would result from the activation of long and pervasive relic fractures. Smaller variations in fracture scale and frequency are not quite so dramatic, and an appropriate balance between spacing and scale may be capable of optimizing the relationship between the efficiency of thermal transfer and the rate of fluid circulation. Observed behavior indicates that stress-enhanced dissolution, initially at equilibrium within the reservoir, may be reactivated as fractures are forced out of equilibrium during hydraulic fracturing. At the conditions examined (250°C reservoir with 70°C injection), however, shear dilation exerts dominant control over changes to permeability.

Part II: Natural Environments

Volcanic dome collapse is an important feature in the life cycle of silicic volcanoes, and can spawn hazardous and highly mobile pyroclastic flows. A number of mechanisms may be responsible for structural failure of volcanic domes, such as dome over-steepening and interior gas pressurization. The Soufrière Hills Volcano (SHV, Montserrat, WI), in common with other volcanoes such as Mount St. Helens, Merapi (Indonesia), and Unzen (Japan), has experienced a number of collapse events coinciding with intense rainfall. In several cases, these events have occurred during periods of residual volcanic
activity, or without precursory seismic signals: Common indicators of failure by traditional mechanisms. Utilizing a several year history of rainfall, seismic, and magma efflux records, Chapter V develops a limit-equilibrium model for rainfall infiltration into a hot lava carapace is developed to evolve stability of the dome at SHV. Dome rocks are cooled by episodic rain infiltration and climatic cooling. Rainfall infiltrates fractures that develop in the hot dome carapace, occludes the void space, and staunches effusive gas flow. Gas pressures build in cracks blocked-off by rain, and may destabilize the dome. The effects of dome growth, heating by magma infusion, and cooling by rain infiltration and climatic influences, are combined to follow the growth of the dome towards ultimate collapse. The model is able to replicate, to reasonable accuracy, the collapse events that are observed, including the triggering of collapse by rainfall events. The principal influence in driving the dome to failure is the evolving geometry in bringing the dome to a condition of metastability. The extreme rainfall events are able to trigger failure, but only when the dome flank is first primed for failure.

Chapter VI continues the application to volcanic environments. Continuous and highly resolved geodetic and efflux records are available for only a few volcanoes. One of those is Soufrière Hills Volcano (SHV), which has been erupting since 1995. Histories of magma efflux and surface deformation are utilized to geodetically image magma transfer within the deep crustal plumbing system. Magma efflux is constrained with wide-aperture geodetic data to supplement a well-documented extrusion record, and uses these to explore the role of deeply sourced fluxes on short-term eruption periodicity. For a model of two stacked magma reservoirs surface efflux and GPS station velocities are co-inverted to recover rates of crustal magma transfer throughout the 12 year duration of the SHV eruption. For each of three eruptive episodes over 12 years, co-inversion of the geodetic and efflux data show that the surface efflux responds to volume/pressure changes at a deep level – rather than a result of simply deflation of a shallow reservoir, as usually presumed. Over this period the lower chamber has deflated stepwise by $\sim 320 \times 10^6$ m$^3$, while the upper reservoir inflated by $8 \times 10^6$ m$^3$. This net deflation of the system of $\sim 320 \times 10^6$ m$^3$ is about one-third of the total effusion of $\sim 0.9$ km$^3$ recorded to date, requiring that the remainder of the magma ($\sim 570 \times 10^6$ m$^3$) has been sourced from below the lower reservoir. These observations may be compared with models that represent the efflux history from a deflating spherical chamber in an elastic medium. This matches the average deflationary history and yields a predicted ultimate eruptive volume of $338 \times 10^6$ m$^3$ from the lower chamber with $\sim 320 \times 10^6$ m$^3$ (~95%) transferred as of March 2007.
Chapter I: Numerical simulation of thermal-hydrologic-mechanical-chemical processes in deformable, fractured porous media

A method is introduced to couple the multiphase, multi-component, non-isothermal, reactive transport, and mineral reaction capabilities of TOUGHREACT with the stress/deformation analyses of FLAC\textsuperscript{3D} to examine THMC processes in deformable, fractured porous media (Figure 1.1). The combined influence of stress-driven asperity dissolution, thermal-hydro-mechanical asperity compaction/dilation, and mineral precipitation/dissolution alter the permeability of fractures during thermal, hydraulic, and chemical stimulation. Mechanical and chemo-mechanical aperture change is governed by an empirical relationship for arbitrary conditions of temperature, $T$, and effective stress, $\sigma'$, \cite{Min et al., 2008},

$$b = b' + b^\text{max} \exp(-\omega \sigma') \exp(-\sigma'(\beta - \chi / T))\quad (1.1)$$

that represents fracture aperture, $b$, as a function of the residual aperture, $b'$, the potential aperture change, $b^\text{max}$, and the coefficients $\omega$, $\beta$, and $\chi$. Slight adjustments are enacted to allow this relationship to exhibit hysteresis. Changes in aperture occurring here are fed back to the mechanical system as equivalent chemical strain. Mass transport of chemical species occurs by advection and diffusion within a dual porosity flow system, with mineral reaction rate governed by \cite{Lasaga, 1984},

$$r_m = \text{sgn} \left( \log \left( \frac{Q_m}{K_m^e} \right) \right) \frac{k_m^T}{A_m} \left[ 1 - \left( \frac{Q_m}{K_m^e} \right) \right] \quad (1.2)$$

for the reaction quotient, $Q_m$, equilibrium constant, $K_m^e$, reactive surface area, $A_m$, and the temperature dependent rate constant, $k_m^T$. Mineral mass is removed or added to fracture and/or matrix volume fractions, occluding or enhancing permeability. The flow system follows a dual-porosity, two continuum structure, while the pressure-mechanical coupling is treated as an undrained system. Fracture and matrix are mechanically linked through linear, dual-porosity poroelasticity, to define the relationship between increment of fluid content, $\delta \zeta^f$, and fluid pressure, $\delta p^f$, as

$$\begin{pmatrix} \delta e \\ \delta \zeta^f \\ \delta \zeta^m \end{pmatrix} = \begin{pmatrix} c_{11} & c_{12} & c_{13} \\ c_{21} & c_{22} & c_{23} \\ c_{31} & c_{32} & c_{33} \end{pmatrix} \begin{pmatrix} -\delta \sigma \\ -\delta p^f \\ -\delta p^m \end{pmatrix} \quad (1.3)$$

for the coupling coefficients, $c_{ij}$, and superscripts for fracture and matrix. The pressure response within the fracture and matrix, respectively, to an incremental change in stress occurs via Skempton coefficients for each domain, \cite{Berryman and Wang, 1995}.
\[
\delta p' = B' \delta \sigma = -\frac{c_{12}}{c_{22}} \delta \sigma \\
\delta p'' = B'' \delta \sigma = -\frac{c_{11}}{c_{33}} \delta \sigma
\]

(1.4)

In a single iteration, fluid pressure builds separately in the two domains, fracture and matrix, in response to a given mechanical strain, and this pressure is dissipated through the next iteration with the dual-porosity flow response of TOUGHREACT, with a correction to enforce conservation of fluid mass. Thermodynamics (compressibility) of water mixtures is provided by incorporation of the 1997 IAPWS steam table equations into the interpolation module (see Figure 1.1). The stress/strain relationship is thus modified, for a linear elastic system, based on two fluid pressures,

\[
\sigma_y = 2G \varepsilon_y + \frac{2G'\nu}{1-2\nu} \delta_y - \left(\alpha_p p' + \alpha_m p''\right) \delta_y - \alpha_T \delta_y
\]

(1.5)

for the coupling coefficients, \(\alpha_p^{(i)}\) and \(\alpha_T\). Analytical comparisons confirm the capability of the model to represent the rapid, undrained response of the fluid-mechanical system to mechanical loading in both fluid pressure (Figure 1.2A) and deformation (Figure 1.2B).

A full thermal loading/unloading cycle of a constrained fractured mass is examined to follow the irreversible alteration of in situ stress and permeability resulting from both mechanical and chemical effects (Figure 1.3). Chemical strain is defined here as thermo-chemo-mechanically irreversible reduction in fracture aperture that results in a relaxation of stress in the surrounding rock. It is proposed to be of significant importance in fractured reservoirs and replicating it one of the primary goals of THMC modeling. Figure 1.3A is the baseline case, with completely reversible permeability change and no feedback of this chemical strain on the stress field. Figure 1.3B represents the case of complete permeability constitutive treatment and includes feedback on the stress field. Figure 1.3C maintains full permeability constitutive treatment (as in Figure 1.3B), but now does not include feedback on stress. Figure 1.3D considers complete reversibility (as in Figure 1.3A), but includes feedback on the stress field. From the figure, the non-linear dependence of aperture on the temperature/stress field is evident, as is the non-linear dependence of stress on temperature that results from the feedback of chemical strain on the stress field. Two-dominant impacts on the system, hysteretic in nature, are visible by comparing the initial, ambient system with the final, ambient system. Importantly, when the system returns to its initial state, there has been an irreversible reduction in the stress field as well as an irreversible decrease in permeability. Neither of these occurrences, intuitively operative and significant in natural systems, may be represented without the inclusion of thermal, hydrologic, mechanical, and chemical processes.

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Figure 1.1 - Coupling relationship between TOUGHREACT, FLAC$^{3D}$, and the interpolation module.
Figure 1.2 - Comparison of TOUGHREACT- FLAC$^{3D}$ fluid-mechanical coupling simulation versus analytical results in 1-dimension. **A.** Normalized ($p_0 = p(z,0) = B_0^\theta \sigma_0$) pressure diffusion response versus diffusive time ($t_D = ct/L^2$). **B.** Normalized ($u_e = u(0,\infty) = \sigma_e L / \lambda^{0.5}$) displacement response versus diffusive time.
Figure 1.3 - Thermal loading/unloading cycle examining the effects of chemical strain. Parameters: $E = 13 \text{ GPa}$, $\nu = 0.22$, $\alpha_T = 12 \times 10^{-6}$. 
Chapter II: Thermal-hydrologic-mechanical-chemical processes in the evolution of engineered geothermal reservoirs

A prototypical enhanced geothermal system (EGS) is examined for the relative, temporal arrival of hydro-mechanical vs. thermo-mechanical vs. chemical changes in fluid transmission as cold (70°C) water is injected at geochemical disequilibrium within a heated reservoir (275°C) (Figure 2.1). Simulations utilize the THMC numerical simulator developed by [Taron et al., 2009]. In-situ, aqueous concentrations are obtained by equilibrating a typical granodiorite mineral assemblage with the conditions of the reservoir. Injection fluid concentrations are obtained by extracting the equilibrium, in-situ reservoir fluid at 275°C and allowing it to cool (not in the presence of reactive minerals, as if utilized at the surface with no treatment other than settling) to 70°C while the aqueous components equilibrate and minerals precipitate.

Three different scenarios are examined for injection fluid chemical activity. Change in mineral abundance (volume fraction) within the host rock is presented in Figure 2.2 for 20 years of simulation.

It is of interest, both for overall reservoir evolution and for evaluation of potential hydraulic/chemical stimulations, to observe the temporal onset of the various mechanistic causes: In what stages of the lifespan of a geothermal project is thermal (or chemical or hydraulic) forcing the dominant mechanism for change? Figure 2.3 compares a conceptual model for the possible temporal relationships between THMC processes (A) with simulation results (B). Total aperture change refers to the contribution from all mechanisms and so reflects the observable change in permeability. Also shown is the contribution to total permeability change due to mineral precipitation/dissolution and thermal-hydraulic processes (asperity dissolution via pressure solution and thermal gaping due to cooling). Aperture change is monitored at three locations in the reservoir (2m, 9m, and 49m outward from injection), and each curve at each location represents the contribution of a different process. Temporal behavior is also examined in terms of characteristic times (Figure 2.4). Characteristic relationships are developed for independent processes of hydraulic, thermo-hydraulic, and chemical, and applied to each plot of Figure 2.4.

Figure 2.5 shows permeability change at a cross section between wells. Note the nearly two order of magnitude variability, and the development of a radial barrier of lower permeability approximately 50m outward from injection. Figure 2.5B illustrates more clearly how this barrier corresponds to the re-precipitation of minerals that are dissolved at injection.

The primary justification for a THMC modeling strategy is that there exists a strong coupling between chemical and mechanical effects that cannot be represented by parallel reactive transport and geomechanics simulations. The truth of this assertion, at the conditions explored in this prototypical EGS, is examined in Figure 2.6. By examination of Figure 2.5 it is clear that both reactive transport and
geomechanical (THMC asperity dissolution/dilation) analysis are required to reproduce the observed order of magnitude changes in permeability; with each causing changes at least as large as one order of magnitude. Furthermore, the pressure solution relationship reduces initial permeability from $3 \times 10^{-11}$ m$^2$ to $6.8 \times 10^{-15}$ m$^2$ at in-situ reservoir conditions (this initial drop is not shown in the figures). Therefore, both of these methodologies are important, and both are required to follow reservoir behavior under these prototypical EGS conditions; but this conclusion does not necessarily imply that they must be interlinked.

Figure 2.6 examines this necessity. Figure 2.6A and 2.6B show permeability changes due only to mineral precipitation/dissolution (from an initial value of $6.8 \times 10^{-15}$ m$^2$). Two different line styles represent two different simulations; the first utilizes our coupled THMC scheme, and the second operates under invariant stress (no mechanical equilibration and thus no pressure solution or thermal-mechanical dilation). Therefore, differences between the two simulations indicate shifts in mineral precipitation/dissolution behavior that are caused by changes in the mechanical system. In Figure 2.6A, at 50m to the left of injection, a reactive transport simulation shows that mineral behaviors cause a reduction in permeability from $6.8 \times 10^{-15}$ m$^2$ to $5.4 \times 10^{-15}$ m$^2$, while the coupled THMC simulation shows a drop to $2.3 \times 10^{-15}$ m$^2$, or a 3-fold increase in the amount of permeability occlusion, while 10m to the left of injection shows a 3-fold increase in permeability enhancement.

Figure 2.6C and 2.6D invert the comparison to examine how changes in the chemical system may alter the evolution of mechanics. Here we plot permeability change resulting only from pressure solution/thermo-mechanical gaping, with the same initial value as before. The lines again represent two simulations; one THMC coupled, and a second that does not allow chemical reaction. Therefore, differences between the two simulations indicate shifts in the thermal-mechanical system caused by changes in the chemical system. In Figure 2.6C we again see shifts in pressure solution/thermal dilation that are caused by precipitation/dissolution, but the coupling is not as strong as for the inverse condition in Figure 2.6A. To examine the potential for greater coupling, Figure 2.6D conducts the same simulation but utilizes a more chemically rich injection water. In this case, very large, order of magnitude differences in thermal-mechanical dilation occur when chemical reaction is included.
Figure 2.1 - Initial conditions and geometric layout of EGS reservoir as used in simulations.
Figure 2.2 - A.) Change in mineral abundance (all minerals combined) at 5 and 20 years for each of the three injection compositions. Negative values indicate dissolution (decrease in the solid volume fraction). B.) Behavior of each mineral utilizing water #2. Each curve normalized to its own maximum value: Number beneath each mineral indicates the normalizing value (multiply by this number to obtain the true value of each curve).
Figure 2.3 - A.) Conceptual model of permeability altering processes after Rose [2006]. B.) Contribution of each mechanism to total permeability change in our simulations. Analogous to (A). Changes monitored at 2 m, 9 m, and 49 m from injection. Uses water #2.
Figure 2.4 - Characteristic times of permeability change due to hydraulic, thermal-hydraulic, and chemical mechanisms. Changes monitored at 9 m, 24 m, 49 m, and 129 m from injection. Uses water #2.
Figure 2.5 - Permeability changes using water #2. A.) Total permeability change with distance from injection. B.) Mineral precipitation/dissolution portion and thermal-hydraulic portion of total permeability change in (A). Note the change of scale on the x-axis of (B).
Figure 2.6 - Permeability comparisons for degrees of coupling. A.) Permeability changing due to mineral precipitation/dissolution only: Compares full coupling vs. reactive transport alone (invariant stress, no stress dependent aperture change). B.) Same as (A), versus time. C.) Permeability changing due to pressure solution/thermal dilation only: Compares full coupling vs. exclusion of reactive transport. D.) Same as (C), using water #3 (all others use water #2).
Chapter III: Constraints on compaction rate and equilibrium in the pressure solution creep of quartz aggregates and fractures: Controls of aqueous concentration

Intergranular pressure solution is an important chemo-mechanical creep process in crustal rocks, and its impact has been shown to be potentially significant in fractured reservoirs [Taron and Elsworth, 2009; Taron et al., 2009]. Despite many previous attempts to model the serial pressure solution mechanism, a fully predictive model remains elusive and the mechanism leading to the cessation of pressure solution at some final, non-zero value of porosity remains poorly constrained. In the following, a relationship is developed for implicit coupling of the dissolution-diffusion-precipitation system (Figure 3.1) without requiring the iterative solution of a linear equation system. Implicit control is maintained over aqueous silica concentrations within hydrated solid contacts and in open pore space. The serial processes of intergranular dissolution, diffusion, and pore space precipitation are, respectively,

\[ \dot{m}^{\text{diss}} = k^+ A^{\alpha} a_{\text{SiO}_2} \left( 1 - \frac{\tilde{C}_i}{a_{\text{SiO}_2} C_{eq}} \right) \]  \hspace{1cm} (1.6)

\[ \dot{m}^{\text{diff}} = \frac{8 D_f \omega}{\tau_f} (\tilde{C}_i - \tilde{C}_p) \]  \hspace{1cm} (1.7)

\[ \dot{m}^{\text{prec}} = k^+ A^{\alpha} \left( 1 - \frac{\tilde{C}_p}{C_{eq}} \right) \]  \hspace{1cm} (1.8)

for the mass flux \( \dot{m} \) [mol·s\(^{-1}\)], and where \( k^+ \) is the forward (dissolution) rate constant, \( A^{\alpha} \) is the reaction area (specific to intergranular or pore space), \( C_{eq}^{\alpha} \) is the solubility of aqueous silica at hydrostatic conditions, molecular diffusivity, \( D_f \), is given by the Stokes-Einstein equation, \( \omega \) is grain boundary width, \( \tau_f \) is the tortuosity factor (square of tortuosity), and for the mean concentration \( \tilde{C}_i \), subscripted for intergranular or pore space. Equation (1.7) is the analytical solution of Fick’s law for a radial contact with a constant flux boundary. Equations (1.6) to (1.8) are utilized to generate the mass balance system for intergranular contact and open pore space, with reference to Figure 3.1,

\[ \dot{C}_i V_i = k^+ A^{\alpha} a_{\text{SiO}_2} \left( 1 - \frac{\tilde{C}_i}{a_{\text{SiO}_2} C_{eq}} \right) - D (\tilde{C}_i - \tilde{C}_p) \]  \hspace{1cm} (1.9)

\[ \dot{C}_p V_p = k^+ A^{\alpha} \left( 1 - \frac{\tilde{C}_p}{C_{eq}} \right) + D (\tilde{C}_i - \tilde{C}_p) \]  \hspace{1cm} (1.10)
which, by finite element rearrangement, conforms to a polynomial solution for aqueous concentrations set within a small iterative compaction scheme for arbitrary conditions of temperature, pressure, and mechanical stress.

A form of “critical stress” is formulated to represent the mechanism leading to final, equilibrium compaction. This form is

\[
\sigma_c = \frac{6E_A (1 - T/T_A)}{4V_m}(1 - \phi) \beta_c^2
\]  

so that pressure solution ceases when stress concentrated at solid contacts reaches the value \(\sigma_c\). Constants represent the molar heat of fusion, \(E_A\), melting temperature, \(T_A\), molar volume, \(V_m\), porosity, \(\phi\), and the “burial constant”, \(\beta_c\), representing the relationship between granular interpenetration and the amount of cement deposited around granular contacts at the cessation of compaction. The burial constant is shown by comparison to laboratory experiments to exhibit quadratic dependence on the applied stress, and thus to be independent of other influences.

The complete model is compared to alternative simplifications in Figure 3.2. The calculation sequence presented here is represented by model \(m1\). Model \(m2\) utilizes a simplified parallel dashpot model for the transition from diffusion to dissolution limited regimes, and model \(m3\) uses a common simplified form of equation (1.6) that is independent of aqueous concentration. Models \(m2\) and \(m3\) are identical when dissolution is dominant (Figure 3.2), predict lower compaction rates than \(m1\) in dissolution-dominated conditions and represent a mean behavior in mixed control systems. Figure 3.3 illustrates the sensitivity of important parameters via their impact on porosity (Figure 3.3A,B,C) and corresponding relationship to aqueous concentrations (Figure 3.3D), varying the value of the 25°C rate constant, \(k_{25}\), and the diffusion and film thickness product, \(D_f\). Model results are compared to experimental data [Niemeijer et al., 2002; Van Noort et al., 2008] in Figures 3.4-3.6. Results are quite agreeable across a range of conditions without modification of controlling parameters. The solution is extended for open and closed systems and is applicable to granular media and fractures, differing only in the method defining evolving contact geometry.
Figure 3.1 - Conceptualization of the chemical compaction process; porous media and fractures.
Figure 3.2 - Porosity (A), strain rate (B), and normalized (to hydrostatic solubility) concentration (C,D) for comparison of alternate forms. All cases utilize T=350°C and $\sigma' = 100$MPa. Model m1 is the calculation sequence presented above, m2 is the viscous dashpot model, and m3 is equation (3.30) only.
Figure 3.3 - Comparison of various parameter changes with T=350°C and \( \sigma^* = 100\text{MPa} \).
Figure 3.4 - Comparison of model with data from van Noort et al. [2008a].
Figure 3.5 - Comparison of model with data from Niemeijer et al. [2002].
Figure 3.6 - Comparison of model with data from Niemeijer et al. [2002]. In (A) all parameters are unchanged. In (B) \( \beta_c \) for cpf8 is adjusted by adding 0.2 to equation (3.37).
Chapter IV: Coupled mechanical and chemical processes during fracture compression and shear: Application to heterogeneous engineered geothermal reservoirs

A model is developed to represent mechanical strain, stress-enhanced dissolution, and shear dilation as innately hysteretic and interlinked processes in rough contacting fractures (Figure 4.1). This model is incorporated into a numerical simulator [Taron et al., 2009] designed to examine permeability change and thermal exchange in chemically active and deformable fractured reservoirs (Figure 4.2). Fractures deform normally via contact theory and Boussinesq half-space deformation. The contact-area-based mechanism allows for direct extension to stress dissolution (C-M creep) and shear dilation, based on direct measurement of fracture surfaces (profiles). Figure 4.3 illustrates the character of the combined action of mechanical strain and pressure solution in a rough fracture. As compaction from PS progresses, contact area is increased while the potential length of deformation is decreased. Eventually pressure solution slows to equilibrium, and the final elastic deformation is small. In other words, the process produces a stiff fracture.

A candidate engineered geothermal reservoir system (EGS) is targeted for analysis, similar to that of [Taron and Elsworth, 2009] (Figure 2.1). The new mechanistic model is capable of distinguishing differences between the evolution of fluid transmission characteristics of 1) small scale, closely-spaced fractures and 2) large scale, more widely spaced fractures and their impact on permeability evolution and thermal drawdown within the reservoir. Figure 4.4 illustrates the advancing permeability and temperature field in a heterogeneous reservoir. Note the strong hydraulic gradient between injection and withdrawal, causing a more rapid advance of cold water along this gradient. White vectors in the figure mark locations undergoing shear failure. Permeability varies over nearly three orders of magnitude. Observed behavior indicates that stress-enhanced dissolution, initially at equilibrium within the reservoir, may be reactivated as fractures are forced out of equilibrium during hydraulic fracturing. At the conditions examined (250°C reservoir with 70°C injection), however, shear dilation exerts dominant control over changes to permeability.

Various test conditions are listed in Table 4.1. The presence of longer and more widely-spaced fractures within a reservoir is shown to be potentially significant and capable of causing both hydraulic and thermal short circuiting (Figure 4.5), through the activation of long and pervasive relic fractures. Larger scale fractures (simulation UT3 in Figure 4.5) allow the rapid advance of a field of increasingly large permeability. Smaller variations in fracture scale and frequency are not quite so dramatic (Figure 4.6), and an appropriate balance between spacing and scale may be capable of optimizing the relationship between the efficiency of thermal transfer and the rate of fluid circulation. The impact in generation rate for various test cases is illustrated in Figure 4.7.
Figure 4.1 - Compaction processes: pressure solution and elastic deformation.
Figure 4.2 - Aperture change scheme. $\Delta b_c$ is aperture change due to mineral precipitation/dissolution, calculated from changes to mineral volume fraction exiting from TOUGHREACT.
Figure 4.3 – Combined fracture closure from pressure solution and elastic deformation. Refer to scheme in Figure 4.4. Dashed lines allow pressure solution compaction and exclude any mechanical equilibration.
Figure 4.4 - Temperature (top) and permeability (bottom) evolution for 5-30 years, in all cases utilizing test SS (spatially variable, anisotropic). White vectors indicate locations undergoing shear. Orientation represents the Coulomb yield surface: rotation angle $\alpha = \tan^{-1} \left( \frac{1 + \sin \phi}{1 - \sin \phi} \right)$ from $\sigma_3$. Vector magnitude is scaled relative to shear displacement.
<table>
<thead>
<tr>
<th>Test</th>
<th>$k$ style</th>
<th>$s_d$ [mm]</th>
<th>$s$ [m]</th>
<th>$k^{x,y}$ [$m^2$]</th>
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</thead>
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<tr>
<td>T0</td>
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<td>1.538</td>
<td>1.060</td>
<td>$8.24 \times 10^{-15}$</td>
</tr>
<tr>
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<td>0.513</td>
<td>1.000</td>
<td>$8.24 \times 10^{-15}$</td>
</tr>
<tr>
<td>UT2(^a)</td>
<td>anisotropic</td>
<td>1.538</td>
<td>1.445</td>
<td>$8.24 \times 10^{-18}$</td>
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<tr>
<td>UT3</td>
<td>anisotropic</td>
<td>2.563</td>
<td>7.720</td>
<td>$8.24 \times 10^{-14}$</td>
</tr>
<tr>
<td>SS</td>
<td>anisotropic</td>
<td>1.538</td>
<td>1.451 ± 1.40</td>
<td>4.19 $\times 10^{-15}$ to 2.35 $\times 10^{-13}$</td>
</tr>
</tbody>
</table>

\(^a\) Moderate fracture spacing case, for comparison to T0 and SS.
\(^b\) Initial x-y permeability, minimum and maximum if spatially variable.
\(^c\) In all cases, the mean permeability (over all elements) is $8.24 \times 10^{-15} ± 0.01 \times 10^{-15}$.
\(^d\) Permeability refers to the post equilibration (pressure solution equilibrium obtained) permeability.

Table 4.1 – Variations in test conditions utilized in simulations.
Figure 4.5 - Permeability evolution with distance from injection at select times. Compares small tight fractures (UT1) against moderate fractures (UT2) and larger scale, loosely spaced fractures (UT3).
Figure 4.6 - Transient advance of temperature at three locations within the reservoir between injection and withdrawal. Compares small features of tight spacing (UT1) with moderate features of less frequent spacing (UT2).
Figure 4.7 - Evolution in generation rate for all tests. Insert shows longer term analysis for UT2 and SS.
Chapter V: Mechanisms for rainfall-concurrent lava dome collapses at Soufrière Hills Volcano, 2000-2002

The evolution of rainfall-concurrent dome collapses at Soufrière Hills Volcano is followed using a limit equilibrium model for rain infiltration into a hot lava carapace (Figure 5.1). If the dome and its rubble substrate are either sufficiently cool (<100°C), or a deluge event is of sufficient volume to quench the contacting rock, infiltrating rainwater may saturate the rind and occlude fracture porosity. The infiltration of rainwater, and its vaporization by dome rocks heated by the infusion of magma, may then pressurize fluid within the fracture. Dome temperature is evolved through considerations of climactic air cooling, periodic quenching from precipitation, and magmatic heat supply. The depth of water penetration for a given rainfall event (Figure 5.2) may then be evaluated as a function of precipitation rate and properties of the dome.

Dome geometry is followed from measured values of magma extrusion rate and incremental collapse volumes from 2000-2002. The geometry of Figure 5.1 examines the lowermost portion of the disjointed dome portion of thickness, \( h \), and inclination, \( \alpha \), isolated by fracture spacing, \( s \), which cuts the full depth of the segment. The maximum gas overpressures resulting from staunched gas flow are set by the infiltration depth. This defines the destabilizing forces that may evolve on the unstable segment of an idealized dome flank (Figure 5.1). The isolated block may fail when the pressure-augmented destabilizing forces exceed the pressure-sensitive reduction in strength of the underlying inclined detachment. Instability is indexed by the “factor of safety”, representing the ratio of stabilizing to destabilizing forces. Equilibrium is established for this geometry as the ratio of the stabilizing forces modulated by cohesive strength, \( c \), block weight, \( W \), and friction angle, \( \varphi \), to the destabilizing influence of the back-scarp water, \( F_w \), and vapor, \( F_v \), forces and by the vapor uplift force, \( F_U \), applied to the basal plane. The factor of safety, \( F_s \), can therefore be defined for a unit thickness of slope as,

\[
F_s = \frac{c + (W \cos(\alpha) - F_U) \tan(\varphi)}{W \sin(\alpha) + F_w + F_v}.
\]

A factor of safety of unity implies that the selected collapse geometry is at incipient failure.

Figure 5.3a shows the response where changes in geometry with dome growth and then collapse are accommodated, and Figure 5.3b where the geometry is retained constant. Using consistent parameters, the rainfall deluges of March 2000 and July 2001 are shown to bring the edifice close to failure for both events, but only where the dome geometry is incremented for magma influx (Figure 5.3a). This is an important outcome, as without this morphological consideration, it is not possible to match observed behavior. While the heaviest rainfall episodes produced the deepest spikes in depth penetration and,
subsequently, $F_s$, these occurrences did not necessarily reach below the required value of unity that implies incipient failure when the dome was experiencing a stage of renewal. However, relative to the large $F_s$ immediately post failure ($\sim 3$), the $F_s$ approaches within a few percent of instability ($F_s \sim 1$) around the time of failure.

The short timescale triggers in developing failure may be examined for the near continuous rainfall history record available throughout the July 29-30 2001 collapse. When the same model is applied to this magnified window, the resulting histories of precipitation, reduced displacement, averaged over one minute, and factor of safety are shown in Figure 5.4. The model maintains a general correlation between the reduction in $F_s$ and the occurrence of clusters of seismic events, although the switch from one day averaged to near continuous time rainfall measurements alters the sensitivity of the analysis. At this scale, where tracking morphological changes becomes impossible, there is a difficulty in resolving the influence of individual rainfall events. At the time of the July 2001 high rainfall events, the dome was metastable, and a variety of rainfall events of varying intensities and durations could conceivably trigger failure. This ability appears beyond the resolution of the current model with a difficulty in resolving between various degrees of instability.
Figure 5.1 - [Adapted from Elsworth et al., 2004] Schematics of dome geometry, infiltration into carapace, and stability analysis. (a) Insets show locations of (b) and (c). (b) Infiltrating water penetrates fractures to depth, d, enabled by locally depressed 100 °C isotherm, and builds water pressure to $p = \rho g d$ at infiltration front. (c) Geometrically separated failure block of weight W raised at angle $\alpha$ to shear plane, held by shear resistance S. Existing gas pressures (dark shading) are augmented (light shading) by stanched gas flow, increasing weakening vapor and water pressure forces ($F_V$ and $F_W$, respectively) and vapor uplift force ($F_U$).
Figure 5.2 - Rainfall infiltration depths as a function of initial dome temperature. Note the development of two behaviors characteristic of short time ($t_D$) and long time. Cases of practical interest for Soufrière Hills relate to Zone II, for a typical fracture spacing of 50-100 meters and storm duration of 3 hours with intensity of 25mm/hr.
Figure 5.3 - Factor of safety (Fs) determination for the period January 1, 2000 to November 1, 2002. (a) Rainfall intensity (read top left axis) and Fs (read right axis), where Fs is a function of evolving lobe thickness. (b) Fs as a function of constant lobe thickness. Rainfall intensity recorded by University of East Anglia rain gauges at Hope (5 km northwest of dome).
Figure 5.4 - Chronology of 29 July 2001 collapse. Rainfall (black dashed line, read on lower left axis) recorded at Hope. Reduced displacement (solid black line, read on top left axis) is averaged over all digital stations (see Figure 10) with the signal averaged over one minute. Factor of safety (top solid line, read on right axis) falls below unity, and for several hours through the first eruptive phase, and dips only briefly below unity during the second phase. This brief dip correlates with the strongest seismic signal. Antecedent rainfall began at 08:00 with the heaviest occurring from 21:00 to midnight (07/30).
Chapter VI: Implications of magma transfer between multiple reservoirs on eruption cycling

Volcanic eruptions are episodic despite being supplied by melt at near constant rate. In this chapter, histories of magma efflux and surface deformation are utilized to geodetically image magma transfer within the deep crustal plumbing system of the Soufrière Hills Volcano (SHV). Magma efflux is constrained with wide-aperture geodetic data to supplement a well-documented extrusion record, and uses these to explore the role of deeply sourced fluxes on short-term eruption periodicity. For a model of two stacked magma reservoirs surface efflux and GPS station velocities are co-inverted to recover rates of crustal magma transfer throughout the 12 year duration of the SHV eruption.

Deformations result at the surface from the superposed inflation, or deflation, of both reservoirs. For an elastic system, with an inflating source at \( I \), the radial \((\dot{r}_i)\) and vertical \((\dot{z}_i)\) surface velocities measured at some location \((r'_i; R'_i)\): Figure 6.1) are proportional to the reservoir inflation rate as \(\dot{r}_i = a'_i \dot{V}^i\) or \(\dot{z}_i = b'_i \dot{V}^i\). For the two-reservoir system considered here, the resulting radial velocities measured at locations \(i = 1, 2\) are,

\[
\dot{r}_1 = a'_1 \dot{V}^1 + a''_1 \dot{V}^u \\
\dot{r}_2 = a'_2 \dot{V}^1 + a''_2 \dot{V}^u
\]

(1.2)

where the coefficients linking the surface velocities to inflation rates are recovered from the Mogi solutions for a strain nucleus as \(a'_i = (3/4 \pi)(r'_i / (R'_i)^2)\). This represents the effect of an inflating chamber collapsed to a point within a homogeneous elastic half-space bounded by a horizontal surface, and for a Poisson ratio of \(\nu = 0.25\).

For each of the three eruptive episodes the co-inversion (equation (1.2)) of the geodetic and efflux data show that (Figure 6.2) the surface efflux responds to volume/pressure changes at a deep level – rather than a result of simply deflation of a shallow reservoir, as usually presumed. This is apparent in Figure 6.2A as an increased magma supply from the basement into the lower chamber, coupled with an active deflation of the lower chamber. For the two-chamber model, the additive flux from these two deeper sources issues into, and causes outflow from the shallower chamber and upper magmatic system with little volume loss, comprising almost the entire surface efflux in all three active episodes. The only apparent volumetric loss between the deep magmatic system and the surface is manifested as calculated minor inflations (episode 1) or deflations (episodes 2 & 3) of the upper reservoir. The co-inverted data indicate that the eruptive episodes deplete the lower reservoir only, and not the upper reservoir, which may even inflate slightly as inflow slightly outpaces outflow.
During subsequent periods of pause, the deep reservoir reinflates, but typically at half the rate of its previous depletion. Because periods of repose were typically shorter than the periods of active depletion (i.e. eruption), the deep reservoir is being depleted (deflated) throughout this decade-long episode. The cumulative volume change for the deep reservoir is illustrated in Figure 6.3, indicating that over 12 years the lower chamber has deflated stepwise by ~320×10^{6} m^3, while the upper reservoir inflated by 8×10^{6} m^3. This net deflation of the system of ~320×10^{6} m^3 is about one-third of the total effusion of ~0.9 km^3 recorded to date, requiring that the remainder of the magma (~570×10^{6} m^3) has been sourced from below the lower reservoir.

These observations may be compared with a model representing efflux history from a deflating spherical chamber in an elastic medium. Cumulative volume change with time \( dV(t) \), for a spherical reservoir discharging through a constant diameter conduit may be defined in terms of the total volume change \( dV_t \), the compliance of the combined magma and chamber system, \( \tilde{C} \), and the Poisseeullte resistance of discharge along the conduit \( B \) as

\[
dV(t) = (\tilde{C} \ dP_t) \exp\left(\frac{-Bt}{C}\right) = (dV_t) \exp\left(\frac{-Bt}{C}\right). \tag{1.3}
\]

The compliance of the chamber is given as

\[
\tilde{C}^i = \pi a^3 \left( \frac{1}{G_R} + \frac{4}{3} \frac{1}{K_M} \right) = \frac{\pi a^3}{G_R} C^i
\]

where behavior is modulated by the shear modulus of the rock surrounding the chamber \( G_R \), the bulk modulus of the magma \( K_M \) and the radius of the chamber \( a \). Magma of viscosity \( \mu_M \) discharges through a conduit of radius \( b \) (15m), length \( h \) (12km) as \( B = (\pi d^4)/(8h \mu_M) \). This enables the change in chamber volume to be followed in time.

This model, equation (1.3), matches the average deflationary history, as shown, and yields a predicted ultimate eruptive volume of 338×10^{6} m^3 from the lower chamber with ~320×10^{6} m^3 (~95%) transferred to March 2007 (Figure 6.4). Although the upper reservoir has been interpreted to be voluminous, of the order of a few cubic kilometers, it is apparent that the major changes in magma storage that have supplied the eruption are from depth (>12 km), with the lower reservoir contributing only a third of the erupted volume.
Figure 6.1 - Schematic of the magmatic plumbing system considered here. Adjacent reservoirs $I$ and $II$ are linked by conduits with little magma volume or storage. Inflating reservoir $I$ at volumetric rate $V^I$ results in surface displacement rates in the radial $r_1^I$ and vertical $z_1^I$ measured at location $(r_1^I; R_1^I)$. 
Figure 6.2 - (A) Average inter-chamber, basement supply, and chamber inflation rates recovered from co-inversion of surface efflux and geodetic data for dual chamber geometry (B). Flux rates are in m$^3$/s of dense rock equivalent (DRE) with surface efflux measured and all others calculated. Error bars denote spread from using the longest aperture station (MVO1) with each of SOUF, HARR, WYTD. Chamber volume change rates (red lower; dark blue upper) are positive for deflation. Surface (dark blue), inter-chamber (red/blue), and basement (light blue) fluxes are each positive for upwards flow. Note that inter-chamber flux is equivalent to the sum of lower chamber deflation and basement supply (which passes through the lower chamber). Surface efflux is the sum of upper chamber deflation and inter-chamber transfer (pass-through). (C) Inflation (negative - red) and deflation (positive - blue) rates for each of the upper and lower chambers throughout the three sequences of eruption followed by pause.
Figure 6.3 - Cumulative volume changes for lower reservoir evaluated from the combined geodetic and efflux histories. Modeled depletion is for a spherical chamber within an infinite elastic medium discharging through a vertical conduit. Parameters are as defined in Table B.2 [Chamber radius 1 km; depth 12 km; conduit diameter 30 m; shear modulus of rock 3 GPa; bulk modulus of magma 1.1 GPa; magma viscosity $55 \times 10^6$ Pa.s].
References


