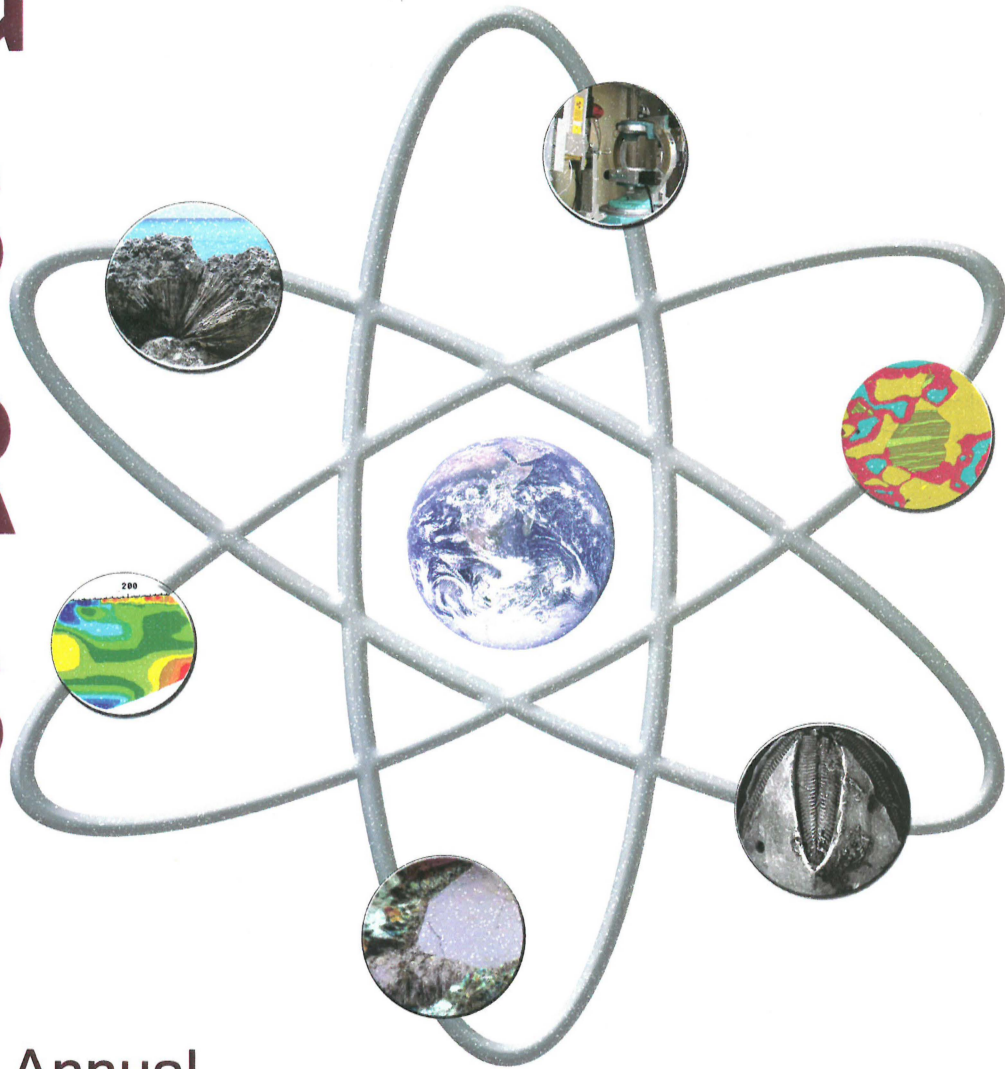


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DEPARTMENT OF
geosciences
AT VIRGINIA TECH



16th Annual
Geosciences Student
Research Symposium
March 3 & 4, 2011

Connecting the World through Geoscience

16th Annual

Geosciences Student Research Symposium

Thursday March 3rd, 2011: 8:45-4:30

Friday March 4th, 2011: 9:00-5:15

4069 Derring Hall

Department of Geosciences, Virginia Tech

Welcome to the Geosciences Student Research Symposium! GSRS is produced and organized by the graduate students of the Department of Geosciences at Virginia Tech. The symposium is designed to allow students the opportunity to prepare and present talks in their current research areas for both professional growth and public awareness.

Constructive feedback on student presentations by faculty, students, and visiting guests is highly encouraged. Evaluation forms will be available at the symposium for those interested. Completed forms should be returned to the boxes provided in the presentation room. Each talk is scheduled to last 12 minutes with three minutes for questions.

Both days of the symposium, breakfasts and light snacks will be served in the 4th floor west lobby, and lunches will be provided in the Geosciences Museum (2062 Derring). A catered dinner in the Geosciences Museum will conclude this year's symposium, and all are welcome to attend.

We are extremely grateful and wish to extend our appreciation to the corporate, local, and alumni sponsors of this event: BP, ConocoPhillips, Schnabel Engineering, Mill Mountain Coffee and Tea, Sycamore Deli, Next Door Bakery, Sub Station II, Zeppoli's and a number of generous alumni! We also thank the Department of Geosciences for their generous support. Finally, to the faculty, volunteers, and student participants, for donating their time and expertise – without you this event would not take place.

Your 2011 GSRS Coordinating Committee:

Committee Chair: Carrie Tyler

Fundraising: Carol Johnson

Abstract Book/Scheduling: Kristie Dorfler, JoBeth Carbaugh, Sarah Timm

Food/Drink: Lindsay Kolbus, Denise Levitan, Tony Giuffre, Ryan Capobianco, Jackie Wittmer, Troy Dexter, Mike Cangialosi

Website: Karina Cheung

Images from the front cover, from top, clockwise:

Lindsay Kolbus: Huber Eulerian 4-circle single crystal X-ray diffractometer; **Kristie Dorfler:** Overlay of Si, Al, Ti, and Mn EDS chemical maps of Salt Hill emery xenolith sample. Spinel (yellow) and Fe-Ti oxides (green striped) are rimmed in garnet (pink). Large Fe-Ti oxide is 100 microns across; **Troy Dexter:** Blastoid pentremites pyriiformis with rare drill hole; **Daniel Moncada:** Quartz crystal showing feathery texture in cross-polarized light; **Jeanne Roningen:** Model electrical resistivity section over northern end of lakebed, Mountain Lake, Giles Co., VA; **Carrie Tyler:** Fossilized Pleistocene coral reef, San Salvador Island, Bahamas. Picture taken during the summer field course: "Taphonomic and Ecological Processes in Tropical Environments", run by Dr. Michal Kowalewski and Dr. Thomas Rothfus (sponsored by the Paleontological Society of America and the Gerace Research Centre).

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CONSTITUENTS OF THE DIELECTRIC RESPONSE: RE-EVALUATING THE ASSUMPTIONS OF TIME DOMAIN REFLECTOMETRY (TDR)

CANGIALOSI, Michael, Dept. of Geosciences, Virginia Tech, Blacksburg, VA 24061

The high electrical permittivity of water makes TDR an attractive geophysical technique for estimating moisture content and characterizing pore fluids. However, partitioning the effects of water and other dielectric materials in the pore-scale hydrologic system remains a challenge to interpreting and applying TDR data. Traditional TDR models assume that the dielectric responses of the individual components in a system do not change when the components are combined. The model expressions that are commonly used to calculate soil moisture content and bulk electrical conductivity overlook the possible influence of soil constituents that affect dielectric responses, and therefore TDR measurements. One example of this problem is seen in studies of partially saturated sandstones, a multicomponent water/rock/air system. Knight and Abad [1995] investigated this system by comparing the dielectric responses of a water-wet and chemically treated hydrophobic sandstone. The two systems produced distinct dielectric responses indicating that two of the components, the water and the rock, interacted strongly to affect the dielectric response. Hence, a careful analysis of the surface chemistry of the grain-scale fluid/rock system has the potential to improve our understanding of dielectric behavior in porous media and decrease uncertainties in interpretations of TDR data. In this presentation I will: 1) summarize the physics of the TDR method 2) show how it relates to current models of fluid/rock surface chemistry, and 3) outline experiments that will explore TDR responses from a model system that is designed to provide a more realistic representation of subsurface geologic environments

Advisors: Dr. P. M. Dove and Dr. C. J. Weiss

CARBON DIOXIDE SEQUESTRATION IN DEEP BRINES: THE VOLUME PROBLEM

CAPOBIANCO, Ryan, Dept. of Geosciences, Virginia Tech, Blacksburg, VA 24061

One of the most significant societal problems we face today is the possible disruption to the Earth's climate and surface chemistry due to rapidly increasing atmospheric CO₂ levels as a consequence of anthropogenic CO₂ emissions. Carbon capture from point sources and sequestration in deep brines is being considered to reduce the impact from fossil fuel combustion. This approach has the potential to sequester CO₂ at a relatively low cost, but there are scientific and technological challenges to implementation.

Carbon dioxide can be trapped in confined aquifers in a free CO₂ phase, dissolved in an aqueous phase (solubility trapping), and as carbonate mineral precipitates. Storage security is enhanced as CO₂ enters the aqueous phase and reacts to form carbonate minerals, but these processes proceed at a slow rate and are anticipated to take decades to centuries to become important in natural systems. In addition, all available pore space in a deep aquifer is already filled with brine, so injection of CO₂ will result in a combination of expansion of the aquifer and increase in pressure. An increase in pressure runs the risk of hydro fracturing the confining layer, which would lead to a loss of CO₂, and aquifer expansion can cause surface deformation. These challenges will likely require pumping, treatment, and disposal of brine to make space for injected CO₂.

Our research has shown that at temperatures and pressures of interest, the apparent molar volume of aqueous CO₂ is roughly half the molar volume of free CO₂. Consequently, storage in the aqueous phase requires about half as much subsurface volume as free CO₂. In addition, CO₂ saturated brine is negatively buoyant so it will sink, enhancing storage security. Increased security and decreased storage volume compared to the free phase make solubility trapping an attractive alternative.

Advisor: Dr. R. J. Bodnar

PETROGRAPHIC AND SUBSURFACE ANALYSIS OF LOWER PENNSYLVANIAN SANDSTONES IN RUSSELL COUNTY, VIRGINIA

CARBAUGH, Joyce, Dept. of Geosciences, Virginia Tech, Blacksburg, VA 24061

In recent years, concern over rising atmospheric CO₂ levels has prompted many researchers to develop strategies for geological carbon sequestration and enhanced hydrocarbon extraction. An enhanced coal-bed methane facility in Russell County, Virginia is targeting lower Pennsylvanian coals for CO₂ storage, but the corresponding coarse sandstone units may also prove to be useful CO₂ reservoirs. This project focuses on the shallowest interspersed sandstone units of the Breathitt Fm in southwestern Virginia, and addresses both petrographic and volumetric analyses in order to assess their reservoir quality.

Lower Pennsylvanian strata in the Central Appalachian Basin have been repeatedly recognized as fluvial sand to coal cap parasequences. The sandstone bodies, which are the focus of this project, vary in composition from quartz arenite to lithic, due to the flux of metamorphic sediments shed from the Appalachian thrust front active during deposition. Complex burial and diagenetic histories of these units have produced considerable amounts of altered and secondary minerals and porosity.

This mineralogical approach to reservoir quality was assessed on both fine and gross scales through detailed petrography as well as regional stratigraphy. Petrographic and scanning electron microscope examination identified and quantified primary and diagenetic grain and matrix mineralogy and porosity. These sandstones have an abundant pseudomatrix of ductile lithic fragments, an average of 6% diagenetic cement, and an average 3% secondary porosity. Permeability thresholds are yet to be determined. Initial work shows a paragenesis consistent with Reed et al. (2005): siderite, ferric oxyhydroxide, chlorite kaolinite, calcite, albite, illite, quartz, porosity, dolomite. Well-logs were used to construct both strike and dip cross sections for 10 km around the core site. The strata exhibit lateral continuity and deepen significantly toward the Alleghanian Thrust Front. A geochemical literature review has supported the aforementioned analyses, focusing on properties of carbon dioxide in combination with water and salts, relevant mineral reactions, and clay dissolution.

At the temperatures and pressures present within these units, CO₂ is unlikely to react with either the primary or diagenetic mineralogy in a way that negatively impacts continued injection on human time scales. The pore volume of these units, given enough permeability, would render them potential reservoirs. Further efforts to characterize the seal capacities are necessary to determine whether the sandstone bodies could operate as failsafe reservoirs for CO₂ in the event the deeper coal-bed seals are compromised.

Advisor: Dr. K. A. Eriksson

USING CRUSTAL THICKNESS MODELING TO STUDY MARS' CRUSTAL/MANTLE STRUCTURES.

CHEUNG, Karina, Dept. of Geosciences, Virginia Tech, Blacksburg, VA 24061

Mars has an intriguing crustal dichotomy that separates the planet into two distinct hemispheres: the Northern Lowlands, characterized by smooth, resurfaced lava plains and low topography, and the Southern Highlands, characterized by rough, heavily-cratered terrain and high topography (Carr, 2006 and Sleep, 1994). The main focus is to find out how Mars got such structures.

Topographic and gravitational potential data can be combined to study the external and internal structures of a planet. Given that the gravitational potential is non-unique, many structural configurations can give the same signature. Thus, a geophysical model is used to study this signature, identifying possible corresponding structures that may have generated that signature (Blakely, 1996).

The model used is a crustal thickness model developed by Mark Wieczorek (2003). It assumes the gravitational potential stems from two sources: surface topography and Moho topography (Wieczorek and Phillips, 1998). When surface topography is accounted for, the remaining gravity anomalies are assumed to come from topography on the Moho. Thus, by varying Mars' crustal thickness, models can be generated to fit the observed gravitational signature.

Crustal thickness and gravity misfit maps are the products of this model. The first experiment involved varying the downward continuation filter to see how the crustal thickness and gravity misfit values change. Specific parameters inputted include a crustal density of 2900 kg/m^3 , a mantle density of 3500 kg/m^3 , and an assumed crustal thickness of 44 km.

For crustal thickness at low degree harmonics ($l = 10$), the model displays the topographic dichotomy and the largest constructs such as Tharsis Rise and Hellas Basin. At high degree ($l = 50$), smaller structures (higher resolution) appear in addition to the larger structures, and an overall thicker crust. A possible mantle plume track also becomes apparent that may have migrated from the South Pole to its current location on the dichotomy boundary (Sramek and Zhong, 2010).

Gravity misfits at low degree ($l = 10$) correspond to the largest structures with large misfit values while at high degree ($l = 50$), the model shows smaller structures with smaller misfit values. Subsequent studies with the incorporation of isostasy and a mantle plume will help us better understand what these crustal thickness and gravity misfit models are revealing about the subsurface and thermal evolution of Mars.

Advisor: Dr. S. D. King

THERMOCHEMICAL PILES: MODELING ELECTROMAGNETIC SIGNATURES TO DETERMINE THE MINERAL MAKEUP OF DEEP EARTH STRUCTURES

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Thousands of kilometers below the Earth's surface, seismologists have discovered massive structures sitting under Africa and the central Pacific. The slower-than-average shear-wave speeds tell us that some sort of anomaly exists, while a lack of correlation in the tomography of long-wavelength shear waves and bulk sound waves indicates that the anomalies stem not from temperature variations, but rather, represent changes in the chemical makeup.

Current efforts to constrain the range of hypothesized thermochemical structures have proven insufficient. Additional constraints and new theoretical approaches are needed. For example, though temperature affects the electrical conductivity of mantle minerals, chemical heterogeneity produces better electrical heterogeneity. This electrical heterogeneity can be mapped directly by using the electromagnetic method. Previous work observing thermally activated conductivity structures gives us reason to believe that the electromagnetic signature due to chemical heterogeneity will also be observable.

Using computational experimentation, we will explore which conditions give rise to electromagnetic observables for various minerals. Earlier global modeling efforts led to the creation of Project MANTIS (the MANTle Induction Simulator), which solves 3D global induction problems. It is geometrically compatible with CitcomS, and it can parallelize via domain decomposition. Initial steps have also been taken to map seismic tomography onto a temperature and composition model to figure out what a large-scale, deep-earth structure would do to the surface magnetic field. Some very basic work has been done to convert temperature and composition fields to a conductivity model, but more work is needed. Using the seismic model, S20RTS, we will create a temperature anomaly field as input for the conductivity model. Since the work is still in the exploratory phase and Earth's physiochemical state in this region remains poorly constrained by current observations, we will use a range of temperatures, densities, and compositional-layer thickness. CitcomS will be used for thermochemical convection experiments, and its compressible formulation can reasonably approximate the adiabatic gradient and viscosity structure.

Ultimately, the goal is to model thermochemical piles similar to those that exist in the lower mantle, but not to replicate the actual piles. Once this is done, we can go back to the observational record and look for the patterns and response-function signatures that will tell us more about the presence and composition of these structures.

Advisor: Dr. S. D. King and Dr. C. J. Weiss

HYDROTHERMAL CIRCULATION AND ICE MELT, A POSSIBLE FORMATION MECHANISM FOR SURFACE MORPHOLOGY ON MARS?

CRAFT, Kathleen, Dept. of Geosciences, Virginia Tech, Blacksburg, VA 24061

Many features on the surface of Mars are believed to have formed by fluid flow. Rovers and orbiters have discovered evidence of water including hydrothermal salt deposits and mineral hydrates at the plateau, Home Plate (Squyres et al., 2008) and subsurface ice indicated by radar observations (Plaut et al., 2009). Similarly to hydrothermal processes on Earth's seafloor, Martian hydrothermal systems may provide a mechanism for transporting water, chemicals, and energy to the surface. These systems could shape surface morphology and may provide environments for biological processes. Therefore, a magma driven hydrothermal system seems a plausible mechanism for forming surface features by causing groundwater release as a result of induced fluid circulation and ice melt.

Here we built upon previous magma driven hydrothermal modeling (Gulick, 1998; Hanna and Phillips, 2006; McKenzie and Nimmo, 1999; Craft et al., 2011) and investigated the amount of fluid provided to the surface by induced circulation and the melting of overlying ice layers. First we modeled a dike driven hydrothermal system with a layer of ice overlying the fluid circulation in the adjacent porous medium. Second, we examined a magmatic sill driven hydrothermal system with an overlying ice layer.

Dike driven system results estimate about 1 km of ice melt over the 3 year lifetime for a 10 m wide, 10 km tall dike with a high $K=10^{-10}$ m² and a 1 km tall, 10 m wide dike with $K=10^{-11}$ m² each, both with μ and α_f parameters at high temperature values. For all other system parameter combinations examined where the steady-state boundary layer theory is applicable, the maximum ice thickness of 2-3 km will melt over the 10s to 1000s year dike lifetimes. With these ice melt contributions, fluid flow rates still remain low for gully formation unless multiple dikes contribute to the formation of one gully. Fluid flow rates for larger systems appear adequate for deltas, fans and valleys. For the ice system overlying a sill, fluid flow rates are estimated at about 0.1 km³/yr for a 1 km² sill surface area, much lower than the estimated required flow rates for surface features. Sill systems could store up melt fluid, however, until finally melting through the ice layer and then release a large volume over a short time. Further work will include examination of rock alteration during the ice melt process and will also consider crystallization of the magma intrusion as it cools.

Advisor: Dr. R. P. Lowell

NANOPARTICLE TRANSPORT IN RIVERINE SYSTEMS: IMPLICATIONS FOR THE ENVIRONMENTAL IMPACT OF NANOTECHNOLOGY, POLLUTANT TRANSPORT AND NATURAL EROSION

DALE, James G., Dept. of Geosciences, Virginia Tech, Blacksburg, VA 24061

Nanoparticles play an important role in natural processes such as pollutant transport and erosional processes. Naturally occurring sediment nanoparticles have been shown to be predominant carriers of pollutants through aqueous systems, while nanoparticle contaminants are known to have increased reactivity and therefore potentially increased toxicity. Understanding the roles of nanoparticles within natural aqueous systems is therefore critical to predicting their posed health threats. Current studies are limited in their scope to pristine systems, making it difficult to extrapolate their findings to environmental systems. This study will examine the effects of colloidal silver nanoparticles, a common commercial nanomaterial and environmental pollutant, through natural riverine media in a laboratory environment.

Benchtop settling experiments will be designed using colloidal silver nanoparticles and well-characterized natural media. Insight into the forces controlling nanoparticle transport through complex media will be gained through utilization of the knowledge and experience of experts in multiple fields. By combining multiple fields such as environmental engineering, chemistry, and hydrogeology, an interdisciplinary approach to developing predictive models of nanoparticle transport will be taken.

Advisor: Dr. M. F. Hochella

APPLICATIONS OF A MOLLUSK RICH FOSSIL ASSEMBLAGE FROM THE PO PLAIN,
ITALY FOR ANSWERING PALEOENVIRONMENTAL AND SEQUENCE
STRATIGRAPHIC QUESTIONS

DEXTER, Troy A., Dept. of Geosciences, Virginia Tech, Blacksburg, VA 24061

Late Quaternary mollusk-rich fossil assemblages from the eastern part of the Po Plain, Italy, were analyzed using multivariate methods to extract paleoenvironmental signals that were then applied to improve sequence stratigraphic interpretations. Spanning 150 ky, eight sampled cores capture two major transgressive-regressive sequences of late Pleistocene and Holocene interglacial intervals and contain fossil assemblages consisting of numerous extant bivalve, gastropod, and scaphopod taxa with known environmental distributions. These cores were densely sampled with 10 cm vertical spacing between samples, and shell material was identified to the species level in each sample. A total of 284 samples have been processed from 8 cores taken at latitudinal and longitudinal transects; and 231 species constituting 120 genera have been identified from a total of nearly 69000 individual specimens. Samples were analyzed via detrended correspondence analysis (DCA), and the resulting DCA scores were calibrated with modern ecological data on extant genera to provide estimates of bathymetry. Depth-related successions of these mollusk associations delineated using DCA were consistent with independent sequence stratigraphic interpretations. The DCA ordination data, calibrated using present-day ecological data, can provide quantitative insights into sequence stratigraphy, including bathymetric and sea-level change estimates, improved interpretation of depositional sequences, and recognition of paleoecological recurrence patterns across comparable systems tracts. Previous analyses were conducted on 3 cores and the patterns are retained reasonably well after data from additional 5 cores have been added. The taxonomic data taken in concordance with sequence stratigraphic information should allow us to develop a regional, 4D reconstruction of the most recent history of this sedimentary basin.

Advisor: Dr. M. J. Kowalewski

MAGMATIC PROCESSES DURING THE FORMATION OF THE ISLAND OF SALINA,
AEOLIAN ISLANDS, ITALY

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The island of Salina is the second largest of the Aeolian Islands, the subaerial expression of the Aeolian Magmatic Arc, an arcuate chain of volcanoes and submarine seamounts, lying north of the island of Sicily, southern Italy. The composition of the erupted products of the arc varies spatially with the western islands (Alicudi and Filicudi) exhibiting a calc-alkaline affinity, suggesting MORB mantle-related genesis and the eastern islands (in particular Vulcano, Lipari and Stromboli) exhibiting calc-alkaline, high-potassium calc-alkaline shoshonitic and alkaline potassic affinities. The island of Salina lies in the centre of the arc and exhibits the widest variation in geochemical composition across all the Aeolian Islands ranging from high-alumina basaltic to dacitic lava flows to rhyolitic pumiceous tephra from 6 different volcanic centers.

Separated by 60,000 years of repose, the Fossa delle Felci and Monte dei Porri cone building eruption cycles occur consecutively in the geological record. Although the stratigraphy is not well defined on Monte dei Porri, a field campaign to sample every unit of Fossa delle Felci and as many distinctly different flows from Monte dei Porri was undertaken in June 2010. These samples will be used in a geochemical study of the evolution of the magmatic system of the islands from the Fossa delle Felci to Monte dei Porri cone-building episodes.

The Monte Porri lava phenocrysts assemblage consists of calcic plagioclase (often with oscillatory zoning), clinopyroxene (augite), olivine and titanium-iron oxides \pm orthopyroxene (clinoenstatite and pigeonite), K-feldspar and quartz. Large mono-mineralic and multi-mineralic glomerocrysts are a common feature of 3 of the 4 samples, as is the presence (in varying degrees) of quartz. The presence of quartz in conjunction with olivine indicates magma mixing may have played a major role in the evolution of the magma during the building Monte Porri. A preliminary study of the Monte dei Porri lavas has revealed the presence of melt and fluid inclusions in the mineral phases. A detailed petrographic study will seek to classify and define the nature and origin of the inclusions. SIMS and FTIR will be used to define the nature of the volatile species and thereby the minimum depth of the magma chamber.

Modeling using the MELTS program will support the petrographic study in determining whether fractional crystallization or the injection and mixing of a fresh magma batch into the system was mostly responsible for the evolution of the system during this transition.

Advisor: [1] Dr. A. Messina; [2] Dr. B. De Vivo; [3] Dr. R. J. Bodnar

QUANTITATIVE STUDY OF DIFFUSION AND CRYSTALLIZATION KINETICS IN UHT CONTACT METAMORPHIC ROCKS

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This research will examine the arrested development of equilibrium textures and mineral compositions in ultra-high temperature (UHT) natural materials in order to test theoretical models and experimental data used to understand inter- and intracrystalline diffusion and crystal growth processes in high-temperature metamorphic rocks. The proposed research will focus on the Salt Hill emery xenoliths of the Cortlandt Complex (CC), expanding upon previous work conducted on the mafic pluton suite of the CC (Friedman, 1956; Barker, 1964; Caporuscio and Morse, 1978; Waldron, 1986; Tracy and McLellan, 1985; Henry, 1997; Johnson and Tracy, 1999; Tracy and Dorfler, 2010). Emery is a mining term for fine-grained, oxide-enriched, Si-depleted metasomatized contact rocks in or adjacent to mafic plutons, i.e. hornfelses. Salt Hill, one of very few emery sites in the world, provides a natural setting to quantify the kinetics of incomplete textural and mineral compositional organization. The emery is an aluminous UHT rock composed of Al-spinel, magnetite, ilmenite-hematite, sillimanite, corundum, Al-rich orthopyroxene, cordierite, sapphirine and garnet, and formed in conditions devoid of fluid during rapid heating to magmatic T ($>1200^{\circ}\text{C}$) at P up to 0.85 GPa, and rapid cooling forming fine-grained rocks with evidence of textural disequilibrium (failure of reactions to go to completion) and very local chemical equilibrium. The hypothesis that local disequilibrium textures and compositions reflect the failure of reaction completion due to limited diffusional transport of components or slow crystal growth kinetics will be tested through the application of theoretical kinetic models of high-T metamorphic reaction pathways to observed textures and measured compositions. An example of textural disequilibrium involves the sequence of silicate rim overgrowths on spinel as local silica activity was raised in Al-rich matrix near quartz veins. The order of silication should be spinel-sapphirine-garnet-orthopyroxene, but spinel crystals may be directly rimmed by any of sapphirine, garnet, orthopyroxene or cordierite with no evidence of production of sillimanite as a necessary reaction byproduct. It is likely that the type of rim growth and the proximal occurrence of these reaction oversteps is due to the controlling factor of diffusive transport of Al away from the reaction site, the Fe/Fe+Mg ratio of spinel (which varies from 0.26 to 0.8, depending on local environment), and the diffusion of Si through the dry matrix. These and other disequilibrium features observed are critical in determining the kinetics of elemental diffusional transport and the chemical reactions that occur at crystal faces.

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DO MELT INCLUSIONS RECORD THE PRE-ERUPTIVE VOLATILE CONTENT OF MAGMAS?

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In the last several decades the number of publications describing the use of melt inclusions (MI) to determine the pre-eruptive volatile contents of magmas has increased significantly. In fact, MI provide the only reliable means of determining the volatile content of the magma before eruption. However, in most MI studies, the volatile contents of the MI vary widely, and it is not possible to assess the reliability of the data. In order for MI to provide reliable information concerning the pre-eruptive volatile content, the MI must obey Roedder's (Sorby's) Rules. Namely, the MI must have trapped a single homogeneous melt phase, the volume of the MI must remain constant after trapping, and nothing can be added or lost from the MI after trapping. In fluid inclusion studies, the adherence to Roedder's Rules is tested by examining two or more fluid inclusions from a Fluid Inclusion Assemblage (FIA), representing a group of FI that were all trapped at the same time. If all of the FI in the assemblage show the same room temperature phase relations and behavior during microthermometry, then it is highly likely that the FI in the assemblage obey Roedder's Rules. A similar approach should be used to study MI, but Melt Inclusion Assemblages (MIA) are rarely studied because they are much more difficult to recognize than FIAs.

In this study, MIAs hosted in phenocrysts from White Island (New Zealand) and from Solchiaro (Italy) were analyzed by Secondary Ion Mass Spectrometry (SIMS). In most MIA, H₂O, F, and Cl abundances were consistent in all MI. However, CO₂ and to a lesser extent S abundances showed wide variation in some MIA, but were consistent in others.

The relatively wide variation in CO₂ content of MI that were presumably all trapped at the same time and location in the magma chamber is problematic. At this time, we do not have a definitive mechanism to explain the variation in CO₂ content for presumably coeval MI, but it could be related to sample contamination from carbon species in the air that were deposited on the sample surface before it was placed into the SIMS, or carbon contamination from acetone used to clean the sample, or other analytical problems. Conversely, the wide range in CO₂ content could reflect complex trapping mechanisms in which the melt becomes saturated in CO₂ during trapping and not all MI are sealed and isolated from the surrounding melt simultaneously.

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CALCIFICATION BY BIOMOLECULE-PROMOTED NUCLEATION AND ASSEMBLY:
NEW ROUTES TO BIOMINERAL FORMATION

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The geoscience community has always accepted that calcium carbonate (CaCO_3) and other biominerals form by traditional crystal growth mechanisms through ion-by-ion addition. Structural biologists, however, have recently shown CaCO_3 skeletons across many phyla form by the accumulation, then transformation of an Amorphous Calcium Carbonate (ACC) phase to crystalline CaCO_3 . For example, an ACC to calcite transformation is observed in the spicules of sea urchin larvae (Politi et al. 2008, *PNAS*). Although the idea of this type of biomineralization is new, its occurrence in diverse organisms suggests the processes are hundreds of millions of years old.

New studies suggest skeletal growth begins by the directed aggregation and transformation of ACC into carbonate biominerals. For example, *in vivo* studies of CaCO_3 biomineralization in crustaceans show a complex biological control on the transformation of ACC to calcitic exoskeletons (Tao et al. 2009, *PNAS*). Evidence suggests biomolecules with specific functional groups such as acidic carboxylates and sulfonates or basic amines have potential to influence the composition of ACC precursors (Raz et al. 2000, *Adv. Mat.*). It also appears that cooperative interactions between the groups create unique chemical environments on organic surface membranes, or templates, that control polymorph and crystal orientation of the mineralized CaCO_3 (Pouget et al. 2009, *Science*). Synergistic interactions between different types of molecules may give new or emergent behaviors that favor the nucleation of biominerals onto substrates (Wallace et al. 2009, *JACS*).

Polysaccharides are one group of molecules of recent interest that may have a potential role in biomineralization. For example, the widely abundant polysaccharide chitin is found at sites of calcification across many phyla in arthropod cuticles, brachiopod shells and mollusk shells (Lowenstam and Weiner, 1989). To investigate the influence of polysaccharides on CaCO_3 mineralization, we are using alginic acid as a simple model compound. This acidic carboxylated polysaccharide is derived from calcifying algae (Bilan and Usov, 2001 *Russian J. Bioorg. Chem.*) and exists in the Extracellular Polymeric Substances (EPS) of stromatolite-forming bacteria. Our initial experiments show that CaCO_3 growth via the ACC pathway is influenced by the concentration of alginic acid in solution as well as the presence of alginic acid films. Future experiments will vary acidic group density along alginic acid chains and investigate the role of chitin films on CaCO_3 nucleation and assembly. Findings from our research may transform how we think about mineral formation in organisms as well as ancient environments where microbial activity was abundant.

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IMPACT OF ASPARTIC ACID ON THE KINETICS OF WATER EXCHANGE ABOUT DIVALENT CATIONS DURING CALCIFICATION

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During biomineralization, aspartic acid (Asp) rich biomolecules influence the nucleation, growth, morphology, structure, and composition of calcified minerals. The mechanism by which these compounds impact calcification may be related to their effects upon cation solvation; dehydration of the cation is considered the rate-limiting step for crystal growth and ion hydration dynamics are thought to be important in mineral growth and dissolution processes. To understand how carboxylated molecules influence the solvation dynamics of cations, we investigated the effect of Asp on the water exchange rates of cations. Two molecular dynamics (MD) methods were employed to calculate hydration water residence times for four biologically relevant divalent cations (Mg^{2+} , Ca^{2+} , Sr^{2+} , Ba^{2+}). Residence times were then recalculated after introducing Asp into the system. All simulations were carried out with the LAMMPS software employing the TIP3P model of water, CHARMM22 force fields, and ion-water potential parameters from Åqvist.

Water residence time calculations reproduce the expected solvation trends based on cation radius. The energy barrier for water escape from the primary hydration shell is greatest for Mg^{2+} and smallest for Ba^{2+} , and water residence times within the first shell increase in the order: $\text{Ba}^{2+} < \text{Sr}^{2+} < \text{Ca}^{2+} < \text{Mg}^{2+}$. In the presence of Asp, formation of contact ion pairs (CIP) and solvent separated pairs (SSIP) between Ca^{2+} , Sr^{2+} or Ba^{2+} and a carboxylate group increases the frequency of exchange for hydration waters. No exchange events for primary sphere waters of Mg^{2+} are observed on the time scale of the simulations, regardless of interaction with Asp. The results demonstrate that soluble biomolecules exhibit kinetic effects upon cation solvation and support the idea that carboxylated molecules promote partial cation dehydration.

Advisor: Dr. P. M. Dove

INSIGHT TO POSSIBLE ENGINEERING SOLUTIONS FOR MANAGEMENT OF
FLUCTUATING LAKE LEVELS AT MOUNTAIN LAKE, GILES COUNTY, VIRGINIA

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Mountain Lake is located in Giles County, in the Valley and Ridge Province of southwestern Virginia. It is one of two naturally formed lakes in Virginia, and the only one located in the southern Appalachians. The lake lies near the top of Salt Pond Mountain ($37^{\circ} 21' 56''$ N, $80^{\circ} 31' 39''$ W), at an elevation of about 1177 meters. At full pond, the lake is approximately 250 meters wide by 900 meters long (Cawley, 2001). Mountain Lake drains and fills periodically, reducing the aesthetic appeal of the property to its patrons. The location of the lake and hotel within a privately-owned nature preserve and adjacent to the federally-designated 16,500 acre Mountain Lake Wilderness, Virginia's second largest wilderness area, gives the hydrologic problem and interesting context: a better understanding of the hydrogeologic system at Mountain Lake will provide useful information for the property owners and those interested in developing geotechnical solutions to the economic problem of fluctuating lake levels (Roning, personal communication).

As Mountain Lake is popular tourist destination, in addition to being a unique hydrologic feature, causing many speculations to evolve offering an explanation as to how the lake formed and why the lake level fluctuates. The surficial geology and geomorphology of the area surrounding Mountain Lake has been documented and mapped, with an emphasis on the sedimentology of colluvium (Mills, 1988). Several others research studies have been conducted to address the question of the lake's geomorphic origin and periodic draining and filling (Parker, 2003). A current study of hydrogeological controls on the fluctuating lake level is being conducted by Roning (MS thesis in preparation). However, there is a dearth of information discussing the lateral extent and sedimentological composition of the deposit damming the lake.

The overall objective of this study is to further characterize the geomorphic origin and hydrological processes affecting the lake's water level from an engineering geology perspective. An understanding of the sedimentological composition and volume of material contained in the dam, combined with evidence of subterranean pathways for water loss, will allow for geotechnical solutions to be evaluated. To address this objective, I will use classical mapping techniques, as well as digital elevation modeling, geophysical methods, and geotechnical analyses to provide a more detailed assessment of the characteristics of the earthen dam.

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