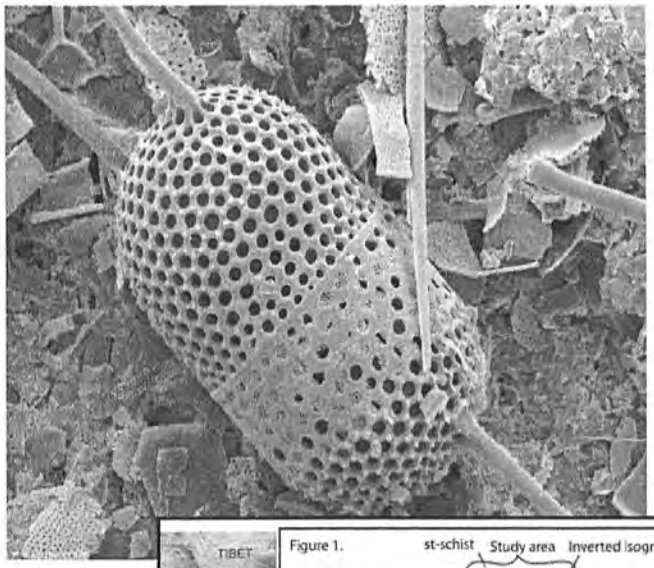
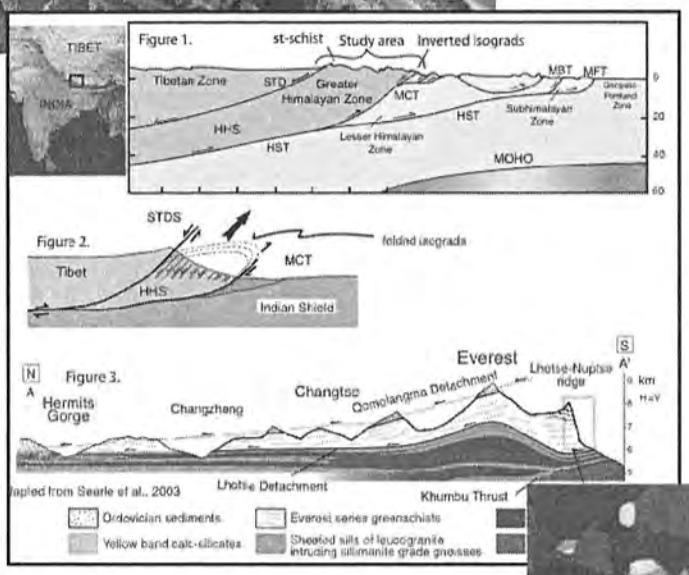
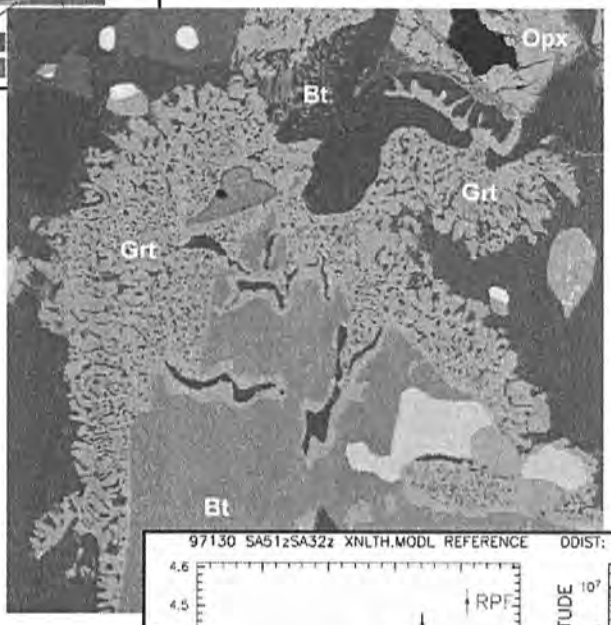
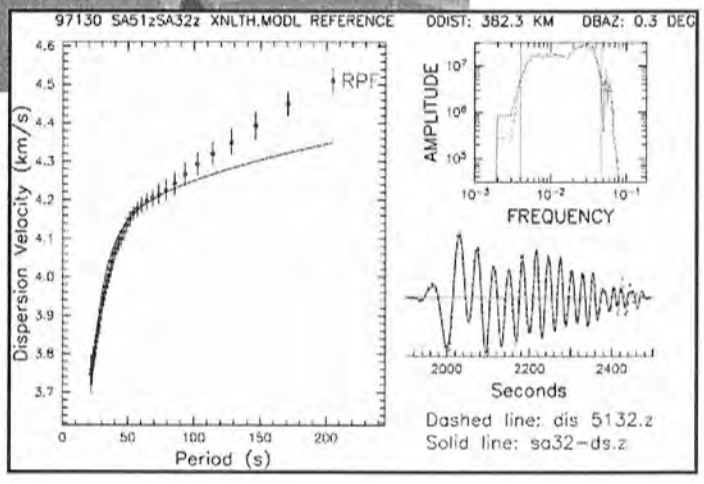


GSSRS 2004

March 18th-19th
Blacksburg, Virginia, USA







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GEOSCIENCES STUDENT RESEARCH SYMPOSIUM 2004

Thursday, March 18th 11:00am – 5:00pm
Friday, March 19th 8:00am – 5:00pm
Derring Hall 4069

The GeoSciences Student Research Symposium (GSSRS) is produced and organized by the students and faculty of the Department of Geosciences at Virginia Tech. The symposium provides an opportunity for the public to learn more about research topics currently being investigated in the geosciences at Tech. It also provides the participating students with an opportunity to prepare and present professional geoscience talks in a friendly atmosphere.

A rotating panel of faculty evaluates student presentations, however, additional comments from students and guests are encouraged as well. Evaluation forms will be available at the symposium for those interested in critiquing the talks and completed forms should be returned to the appropriate location which will be announced during the symposium. The presentations are roughly grouped by level of experience and each talk is scheduled to last twelve minutes with three minutes for questions.

Light snacks and beverages will be available during breaks in 4052 Derring Hall. In addition, lunch will be provided in the Geosciences Museum at 1:45 pm on Thursday, March 18 and also on Friday, March 19, at 12 pm for all speakers, faculty, undergraduate assistants, and department guests. There is also a social and buffet dinner in the Museum on Friday evening at 5:00 pm.

We are extremely grateful and wish to extend our appreciation to the corporate and alumni sponsors of this event: ExxonMobil, ChevronTexaco, ConocoPhillips, the Virginia Tech Department of Geosciences, Andrew Bush, Tracy Cail, Treavor Kendall, Jason Reed, Eric & Maria Rufe, and Shelley E. Tyree. We would also like to thank those faculty members who signed up to evaluate presentations. Your time and support is greatly appreciated.

2004 GSSRS COORDINATING COMMITTEE:

Stephen Becker
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Rocky Severs, Chair

FACULTY ADVISORS:

Dr. R. J. Tracy
Dr. C. Coruh

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5:00 PM	**DINNER**	**DINNER**	

HYDROTHERMAL CRYSTAL GROWTH

NACKLEY, Nicole A., Dept. of Geosciences, Virginia Tech, Blacksburg VA 24061

Hydrothermal crystal growth is utilized for both the scientific and commercial activities. Scientists use hydrothermally-grown crystals to study their structure, and physical properties. The experiments carried out in this project used an ammonium chloride solution to enhance the hydrothermal solubility of calcium carbonate, ferric oxide, ferric-ferrous oxide, and kaolin in order to grow crystals of calcite, hematite, magnetite and kaolinite. Samples were subjected to heating and cooling cycles in hydrothermal autoclaves. At high temperature the NH_4Cl reacts to produce $NH_3(aq)$ and hydrogen ions, thereby producing an acidic solution with high Cl^- activities. This solution increases the solubility of the samples and leads to their recrystallization.

Advisor: Dr. J. D. Rimstidt

COMPRESSIBILITY OF ALBITE, $NaAlSi_3O_8$

BENUSA, Matt, Dept. of Geosciences, Virginia Tech, Blacksburg VA 24061

A study is underway to determine the compressibility and equation of state of low albite, $NaAlSi_3O_8$, using high-pressure single-crystal X-ray diffraction. Low albite is triclinic and belongs to space group C-1. The cell dimensions at room pressure are a=8.1409(8) Å, b=12.7883(5) Å, c=7.1602(7) Å, α=94.251(7)°, β=116.578(7)°, γ=87.676(6)°. An untwinned single crystal of albite was selected for study on the basis of its diffraction quality and loaded in a diamond anvil cell, together with a ruby chip for approximate pressure measurements and a quartz crystal as an internal diffraction pressure standard (Angel et al., 1997). A 4:1 mixture of methanol: ethanol was used as the pressure medium. Thus far, nine pressure-volume data points have been collected between room pressure and 5.859 GPa. A third-order Birch-Murnaghan equation of state fit to these nine pressure-volume data points yields a bulk modulus of 56.5(5) GPa and a pressure derivative of the bulk modulus, K'=3.7(2). An earlier study of low albite to 4 GPa by Downs et al. (1994) found K=54(1) GPa and K'=6(1). The discrepancy in K' probably arises from the different pressure ranges in the two studies. The compression of the structure is anisotropic with the a-axis almost three times as compressible as the b-axis. The c-axis is slightly more compressible than b. The unit cell angles show the following trends between room pressure and 5.9 GPa: α decreases from 94.251(7)° to 94.138(9)°, β increases from 116.578(7)° to 117.099(8)° and γ increases from 87.676(6)° to 88.022(7)°. The compression of low albite will be compared with other feldspars.

Advisors: Dr. N. L. Ross and Dr. R. J. Angel

SEQUENCE SIGNATURE OF A DISTAL FORELAND CARBONATE RAMP DURING GLOBAL GREENHOUSE, ORDOVICIAN, EASTERN U.S. APPALACHIANS

DEMOE, Laura, Dept. of Geosciences, Virginia Tech, Blacksburg, VA, 24061

The middle Ordovician limestone provides a potential window into a carbonate ramp in a tectonically active foreland basin that developed during greenhouse times and is continent collision related. The ramp stratigraphy will evaluate how facies vary and stack during greenhouse-driven sea level changes.

Previous regional work provides large and detailed data sets that include numerous bed-by-bed logs. However, the study predicted high-resolution sequence stratigraphy and generalized complex lithologic successions into simplified facies associations and regionally mapable formations. More recent work in Virginia and Tennessee identified 3 sequences within the super sequences of the Middle Ordovician limestone. Parasequences characterize shallow parts of the ramp succession with a very high frequency and cyclicity. The deep subtidal units show only limited parasequence development and a long period of cyclicity or none. Then the study will document the scales of cyclicty on the greenhouse ramp.

Digitized columns will be constructed in order to create detailed cross sections. These cross sections will display the distribution of facies, parasequences, and sequences, along with bounding surfaces. Stable carbon/ oxygen isotope profiles will be constructed across possible subaerial boundaries. Unpublished diagentic component data suggests that vadose silts show light C isotope values. This means that microbial influences on emergent limestones must have been involved long before land plant development. Computer models will be generated using geological reasonable rates of sedimentation, substance, sea level history, and other variables to constrain the likely sea level durations and amplitudes involved in the formation of the immense greenhouse ramp system.

Advisor: Dr. J. F. Read

CONTINUING RESEARCH ON THE MAGNETIC STRATIGRAPHY OF THE UPPER CRETACEOUS (CAMPANIAN(?)-MAASTRICHTIAN) MAEVARANO FORMATION OF NORTHWESTERN MADAGASCAR

CASEY, Michelle M., Dept. of Geosciences, Virginia Tech, Blacksburg, VA 24061

The Maevarano Formation of Northwestern Madagascar (Mahajanga Basin) is know for its spectacular assemblage of fossil vertebrates including fish, frogs, turtles, crocodyliforms, dinosaurs, birds, mammals and snakes. Correlation with the marine Berivotra Formation (which contains foraminifera of a Maastrichtian age) suggests that the Maevarano Formation is Campanian(?)-Maastrichtian in age. The first ever magnetic study of the Berivotra and all three members of the Maevarano (Anembalemba, Masorobe, and Midana) Formations was conducted using 24 sample horizons (with an average spacing between horizons of 4.4m) and analyzed using alternating field (AF) and thermal demagnetization methods. The study revealed a long normal polarity signal (horizons 1 through 22) capped by a single reversal (the top two sampled horizons). Based on their position relative to the independently defined K/T boundary capping the interval, the normal and reversed intervals are interpreted to represent chrons 30N and 29R, respectively. This suggests a much younger age for the section under scrutiny and is consistent with its taphonomy (excellent preservation indicating rapid burial) and sedimentology (no indications of significant hiatus or erosion). A recent reappraisal of the biostratigraphy of the Berivotra Formation, which linked biostratigraphic zones to predicted magnetic signals for various horizons within the Berivotra Formation, contradicts some of this primary magnetic data. The resulting ambiguities hastened the recent collection of new samples from a number of previously sparsely sampled or disputed horizons and will yield a more precisely defined magnetic signal for the study interval as well as better age constraint for the diverse fauna it yields.

Advisor: Dr. M. Kowalewski

GLACIOEUSTATIC CONTROLS ON PEAT ACCUMULATION: A CASE STUDY FROM THE LOWER PENNSYLVANIAN POCAHONTAS FORMATION, SW VIRGINIA, USA.

BODEK JR., Robert J., Dept. of Geosciences, Virginia Tech, Blacksburg, VA, 24061

The accumulation of coal and its precursor peat has been attributed to many factors. In particular, it has been suggested traditionally that autogenic processes such as channel avulsion and delta lobe switching are major factors in the development of coal beds. More recently, in light of sequence stratigraphy, peat accumulation has been related to allogenic processes such as eustatic changes and climatic variability. In particular, peat accumulation is considered to take place during times of optimal accommodation increase in paralic environments as dictated by eustasy. Coals occurring in a vertical succession within the Lower Pennsylvanian Pocahontas Formation of the central Appalachian Basin were formed during times of global icehouse conditions. If a eustatic mechanism is proposed, then coal beds of the Pocahontas Formation were formed as a function of high magnitude sea level fluctuations. Preliminary interpretation of geophysical wireline logs indicates that coal beds in the Pocahontas Formation cap upward-fining estuarine facies, indicating retrogradational facies stacking associated with a baselevel rise. They also cap upward-coarsening bayhead delta facies, indicating progradation of facies associated with a baselevel fall or increased siliciclastic input. These stratigraphic relationships of coal beds suggest that the initiation, accumulation, and cessation of peat mires were associated with cyclic baselevel fluctuations.

The following project will develop a sequence stratigraphic analysis of coals and related strata of the Pocahontas Formation in southwest Virginia. The initial parts of this project will utilize a GIS database to depict the spatial distribution of coal beds and associated facies in the subsurface. This study will also involve the analysis of a network of geophysical well logs located in the subsurface of Dickenson, Russell, and Wise counties, Virginia, as well as measured sections of outcrop along the nearby Pulaski overthrust. Data from these investigations will be used to construct diagrams depicting stratigraphic relationships in the subsurface. The ultimate goal of this project is to construct a predictive model for the occurrence of coal beds in paralic paleoenvironments.

Advisor: Dr. K. Eriksson

ANALYSIS OF THE ERUPTION OF MT. ETNA, ITALY, DURING SUMMER 2001 AND EVIDENCE FOR THE INTRUSION OF DIKES BY GEOPHYSICAL AND SEISMOLOGICAL COMPUTATIONS

CANNATELLI Claudia, Dipartimento di Geofisica e Vulcanologia, University of Naples "Federico II", Naples, Italy

In the summer of 2001, from July 17th to August 9th, a complex eruption occurred on Mt. Etna volcano (Sicily, Italy) with 50 million km^3 of erupted lava and duration of 23 days. This eruption was very unique because of the simultaneous occurrence of a summit eruption with a lateral eruption on the southern flank of the volcano. A preliminary examination of the erupted products showed many inclusions of sedimentary material that probably originated 500,000 years ago, during an extremely explosive period for the Etna volcano.

Work to characterize Etna's eruption during July-August 2001 includes: 1) computing the stress field and the deformation that occurred with the rising of two dikes, one at 2100-2500 m above sea level and the other at 2700 m above sea level, 2) description of a physical model for these dikes and analysis of the seismic signal before, during and after the eruption period. From the computed deformation it was possible to understand the geometry of each dike and to establish their dimensions; from the analysis of the seismic signal it was possible to link changes in the signal with changes in the source of the signal, and to associate it with the temporal evolution of the eruption.

Advisors: Dr. B. De Vivo and Dr. R. J. Bodnar

SEISMIC RESOLUTION OF THE COAST PLUTONIC COMPLEX (CPC) IN BRITISH COLUMBIA

SHUMAKER, ADAM, N. Dept. of Geosciences, Virginia Tech, Blacksburg, VA 24061

Crustal fractionation is thought to occur via bimodal magmatism under collisional arcs. Partial melting of the mantle produces basaltic melts, whereas the composition of the crust is intermediate. Repeated episodes of plutonic magmatism beneath arc environments during orogenic episodes are thought to fractionate the crust into a feldspathic upper suite and an ultramafic lower suite. Gravitational instabilities may facilitate a detachment of the ultramafic root, which would diapirically sink back into the mantle. A seismic wide-angle refraction/reflection survey across the CPC will play an integral role in finding the ultramafic root. Although an ultramafic root would be seismically indistinguishable from the upper mantle, the imaging of the upper crust will provide volumetric constraints on the putative size of the ultramafic residue. The ultramafic root can only be detected by its anomalously high gravity signature in the upper mantle. Therefore, a robust model of the upper crust is required to accurately constrain density gradients in the lower crust or upper mantle.

Advisor: Dr. J. A. Hole

SECULAR PATTERNS IN MORPHOLOGICAL DISPARITY AND BODY SIZE OF ACRITARCHS THROUGH THE NEOPROTEROZOIC AND EARLY CAMBRIAN

HUNTLEY, John W., Dept. of Geosciences, Virginia Tech, Blacksburg, VA 24061

Acritarchs are a group of phylogenetically heterogeneous microfossils that are interpreted as the resting cysts of eukaryotes. Their diversity through the Neoproterozoic and early Cambrian has been estimated by counting species. These estimates suggest that diversity increased steadily in the early Neoproterozoic and then decreased sharply between 700 and 600 Ma, a drop likely related to Neoproterozoic glaciations. An ephemeral diversification of process-bearing acritarchs (acanthomorphs) followed the glaciations, but many of these acanthomorphs disappeared in Ediacaran time. Acritarch species diversity increased again in the early Cambrian. Anecdotal evidence also suggests that acritarch size and complexity increased throughout the Neoproterozoic until the Ediacaran extinction, and that post-Ediacaran acritarchs reached the levels of morphological complexity, but not the large sizes, recorded for the Neoproterozoic.

This reconstruction of the evolutionary history of acritarchs has recently been brought into question, due to severe inconsistencies associated with acritarch taxonomy. We propose an independent strategy for investigating the evolutionary history of these early eukaryotes, by analyzing size and morphological complexity of acritarchs using quantitative data obtained from the literature. This method is not affected by the taxonomic problems of naming and counting species. Data are being assembled from monographs on Neoproterozoic to early Cambrian acritarchs. Size and morphologic data collected include: vesicle size and morphology, process size, morphology, and count, presence/absence of enveloping membranes, and excystment structures. Other data collected include: paleogeographic location, best estimated age, lithology, depositional environment, mode of preservation, and preparation technique. The resulting dataset is explored using multivariate and computer-intensive methods.

Preliminary data do not suggest any significant changes in acritarch vesicle size between 720 and 580 Ma. Moreover, Multidimensional Scaling based on morphological characters does not suggest any major shifts within the occupied morphospace through this time interval. These pilot results should be interpreted with caution until more data are available.

Advisor: Dr. M. Kowalewski

ENGAGING INTRODUCTORY GEOLOGY STUDENTS WITH DATA: COMPARING AND CONTRASTING THE IMPACT OF DIFFERENT DATA TYPES ON STUDENT LEARNING IN THE LABORATORY CLASSROOM

LUKES, Laura A., Department of Geosciences, Virginia Tech, Blacksburg, VA 24061

Organizations, such as the Digital Library for Earth Systems Education (DLESE), are implicitly operating on the assumption that data-rich experiences in the earth science classroom beneficially facilitate student learning of both content knowledge and the nature of earth science. However, as the NSF Geoscience Education Initiatives of 1998-9, from which DLESE was initially funded, point out (see Geoscience Education, A Recommended Strategy Report), uncertainty exists about how students learn the geosciences at any level and which practices are more effective. Currently, a data-rich classroom experience has been defined rather broadly by DLESE to include the use of raw, derived and/or simulated data (www.dlese.org "Using Data in the Classroom"), making it unclear which types of data are the most effective tools to use in data-rich experiences.

In general, there are two end member types of data: real and contrived. The difference between the two data types lies in their method of construction and their intended purposes. Real data are data that have been collected in order to investigate something; these data contain outliers, errors, and variability. Commonly, scientific practitioners interpret these data to create models for how the world works. That is to say, a model depends directly on the results of the data. Contrived data are either real data that have been simplified or streamlined or are data that have been created altogether, both with the purpose of illustrating a desired concept or model. Commonly, contrived data are used to illustrate how (well) the world works according to a previously established model. That is to say, the data are contrived such that they illustrate or support the model.

These inherent differences in purpose can potentially limit the data's usefulness in communicating the nature of science and/or content material to students. Addressing the subjective, creative, and uncertain nature of science is unavoidable with the use of real data and leads students to their own non-absolute conclusions. These aspects of science essentially are eliminated with the use of contrived data, unless the data is contrived in such a way to specifically address these issues. This raises concerns about the effectiveness of contrived data-rich experiences in communicating the nature of science to students, particularly since many teachers use contrived data almost exclusively.

The overall goal of this project is to provide both quantitative and qualitative evidence that can be used to constrain the definition of an effective data-rich experience in reference to earth science education and suggest effective ways to use real data in established curricula. To test the effectiveness of these two data types, we have created two two-week lab modules based on the two data types. In both modules, students study how the San Andreas fault zone behaves tectonically. In the real-data-based module, students use offset and uplift data to explain how the San Andreas behaves. In the contrived-data-based module, students use contrived data to show that the San Andreas is undergoing transpression. The real-data-based module was offered as an exercise during the 2003 Fall term in 12 of the 21 physical geology lab sections. The remaining lab sections acted as a control group and worked through the existing lab module, a capstone geological mapping exercise, which addresses neither the content nor the nature of science issues addressed and tested for by the experimental modules. In Spring 2004, both the real-data-based and contrived-data-based modules will be offered in all 9 sections of lab. Preliminary results suggest that, despite an apparent testing effect, students engaged with real data gain in both their understanding of the nature of science (2.18 % mean score increase after removing testing effect) and content (41.3% increase in mean content scores after removing testing effect).

Advisors: Dr. B. Bekken, Dr. S. C. Eriksson, & Dr. J. A. Spotila

GEOCHEMICAL INFLUENCES ON CONTAMINANT FATE: A STUDY IN ALMA, MICHIGAN

LEARMAN, Deric R., Dept. of Geosciences, Virginia Tech, Blacksburg, VA 24061

For many decades, the east side of Alma, Michigan has been home to an oil refinery. Local citizens are concerned by the existence of a benzene plume and petroleum contamination in the surface aquifer. Although governmental agencies are working to clean up the refinery site, an unresolved aspect of the problem is whether groundwater is transporting contaminants to the nearby Pine River.

The hypothesis investigated is that contamination from the refinery has affected the quality of groundwater discharging to the Pine River. Groundwater, river water, and sediment samples were analyzed for heavy metals that are associated with crude oil and petroleum refining operations.

The results show heavy metal concentrations in the river and groundwater are presently not transporting significant amounts of contamination. The groundwater and sediments, however, both show elevated metal concentrations in the sampling sites directly down gradient from the refinery. Because of the high sediment concentrations and the lower values of surface water and groundwater, it is concluded that this area was a former path for the contamination plume from the refinery.

Advisor: Dr. M. F. Hochella, Jr

KINETICS OF SCORODITE DISSOLUTION

HARVEY, Mary, Dept. of Geosciences, Virginia Tech, Blacksburg, VA 24061

Scorodite ($FeAsO_4*2H_2O$) is a common weathering product of arsenopyrite (FeAsS), one of the main arsenic-bearing minerals in the earth's crust. Because scorodite is more soluble than arsenopyrite under low pH conditions, its dissolution rate can potentially exert strong control on arsenic release from arsenopyrite oxidation. Previous studies have focused on the stability of scorodite (Dove and Rimstidt 1985) and on methods for precipitating scorodite to remove arsenic waste from mine waste (Demopoulos, 1995). However, little is known about the dissolution kinetics of scorodite.

In this study, the dissolution rate of scorodite will be determined as a function of temperature (15, 25 and 35 degrees Celsius). Experiments will be conducted using a batch reactor design in a controlled temperature water bath. Samples will be analyzed for iron and arsenic over time. The initial rate method will be used to estimate the scorodite dissolution rate. The scorodite dissolution rate can then be used in geochemical transport simulations to assess controls on arsenic release and transport within natural waters.

Advisor: Dr. M. E. Schreiber

PALEOGEOGRAPHIC RECONSTRUCTION OF A TRUNK-TRIBUTARY FLUVIAL SYSTEM, LOWER PENNSYLVANIAN LEE FORMATION, SW VIRGINIA

BENSON, David C., Dept. of Geosciences, Virginia Tech, Blacksburg, VA., 24061

The purpose of this research is to develop a new, genetic sequence stratigraphic framework for the Lower Pennsylvanian Lee Formation and equivalent strata of the Central Appalachian Basin. The hypothesis is to test and further refine recent work done on the New River Formation in West Virginia (equivalent strata). This study identified erosionally-based, tabular and lenticular sandstone bodies of fluvial-estuarine origin comprising an extensive trunk-tributary paleovalley system and postulated that penecontemporaneous tectonic (thrust loading) and glacioeustatic signals (high magnitude sea level changes) controlled sequence development. Depositional models of the spatially similar Cretaceous western interior foreland basin valley fills showed that fluvial sandsheets are attached to proximal facies and grade basinward to marginal marine facies. This model does not account for the sequence architecture previously reported for the New River Formation where fluvial sandsheets are part of the distal foreland basin fill, and interfinger towards the thrust front with fine-grained marginal marine and subordinate nonmarine strata. A new depositional model must be developed to account for these variations.

This study will comprise substantial field work and laboratory analysis. Opportunities for extensive field mapping of the Lower Pennsylvanian Lee Formation are available at Breaks Interstate Park, located in SW Virginia. Measured stratigraphic sections, detailed sedimentology, petrography, and paleocurrent analysis will be performed at various outcrop localities within and adjacent to the park. This data set will not only provide the needed sedimentological evidence for a new genetic model, but will also aid the interpretation of subsurface data. Subsurface data will come primarily from electrical logs (gamma ray and density), supplied by the Virginia Department of Mines, Minerals and Energy, from coal bed methane exploration in the region. These will be digitized, compiled, and correlated spatially within a GIS framework in order to reconstruct, spatially and chronologically, the paleogeography of the Lee Formation. In particular, coal beds will be used as datums to construct time-slice paleogeographic maps showing the spatial distribution of facies/depositional environments.

Sequence stratigraphy has proven to be a powerful tool in resolving the marine stratigraphic record and understanding the complex interplay between tectonics, eustasy, and climate. However, the relationship between these controls and the nonmarine stratigraphic record remains controversial. This study provides an excellent opportunity to assess extrinsic controls on sequence development in a foreland basin setting due to the wealth of subsurface and outcrop data available.

Advisor: Dr. K. A. Eriksson

KINEMATIC AND THERMAL EVOLUTION OF THE HIGH HIMALAYAN SLAB, EVEREST MASSIF, TIBET AND NEPAL.

JESSUP, M.J. Dept. of Geociences, Virginia Tech, Blacksburg, VA 24061

The north-dipping metamorphic and anatectic core of the Himalaya, known as the High Himalayan Slab (HHS), extends for ~ 3000 km along strike and, in central Nepal, is bounded to the south (bottom) and north (top) by the Main Central Thrust (MCT) and South Tibetan Detachment System (STDS) respectively (Fig. 1; Hodges, 2000). Assuming simultaneous movement on the MCT and STDS, the slab can be modeled as a southward extruding wedge or slab of deep crustal rocks (Fig. 2; Hodges, 2000). The general geometries and timing of movement along the MCT and STDS, as well as P/T/t paths within the lower to middle sections of the slab, are fairly well constrained. Critical gaps, however, remain in our understanding of the distribution of strain and metamorphic isograds within the HHS; two aspects with profound implications for the geologic evolution of the Himalayas.

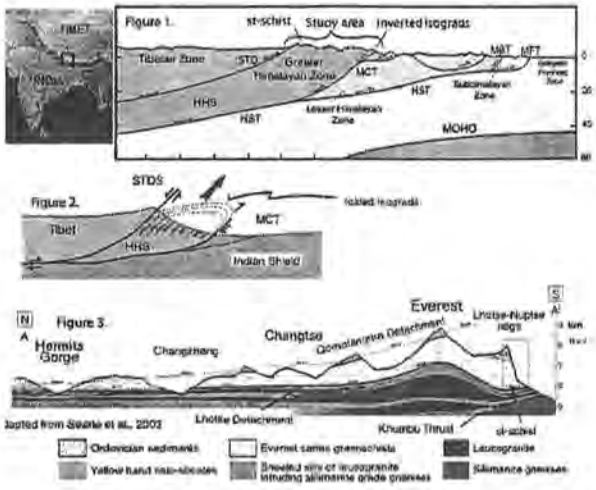

Figure 1. Idealized cross section of the Himalayan collision zone. South Tibetan Detachment (STD); Main Central Thrust (MCT); Main Boundary Thrust (MBT); Main Frontal Thrust (MFT). Hodges, 2000. Figure 2. Extrusion of the HHS proposed by Grujic et al., 1996. Notice the use of inverted isograds. Figure 3. N-S cross section through Mount Everest and the Lhotse/Nuptse ridge. St-schist highlighted by box. Adapted from Searle et al., (2003).

Results from 175 samples collected from the north and south sides of Mount Everest have enticing kinematic and thermal implications. Petrofabric results from greenschist to sillimanite grade metasedimentary rocks at the top of the slab exposed in the Rongbuk Valley, Tibet, show the following: Type I and II cross-girdle c-axis fabrics imply plain strain conditions; 2) Progressive increase in opening angle with depth suggests an increase in deformation temperatures from ~625° to 450°C; 3) Mean kinematic vorticity number (Wm) range from 0.67-0.98 indicate dominantly simple shear with a component of pure shear deformation. In addition, petrography on samples from pristine staurolite schist in talus at the base of the 3.5 km high Lhotse/Nuptse wall marks a decrease (~550-650°C) in metamorphic grade in the upper section of the HHS (Fig. 4). Together these results shed light on the relationship between deformation, anatexis and polyphase metamorphism during the evolution of the High Himalayan Slab.

Advisor: Dr. R. D. Law

QUANTITATIVE ANALYSIS OF EARLY PERMIAN FUSULINIDS

DONG, Lin, Dept. of Geosciences, Virginia Tech, Blacksburg, VA 24061

Fusulinids are extinct foraminifers that occur abundantly in late Paleozoic shallow-water carbonates. In this study, I use several statistical methods to quantify the morphology of Early Permian fusulinid tests, in order to shed light on the ontogeny, taxonomy, and paleoecology of these fusulinids. My analysis shows that (1) the spirotheca of fusulinid test thickens during ontogeny; (2) spirotheca thickness and number of volutions are not diagnostic taxonomic features at the generic level; instead, septum morphology is a better taxonomic feature; (3) variations in spirotheca thickness and number of volutions are associated with sedimentary environments.

Coupled paleoenvironmental and morphological analysis indicates that the most important factor controlling spirotheca thickness is hydrodynamic energy. Larger fusulinid tests have to endure greater hydrodynamic forces, partially explaining the ontogenetic trajectory of spirotheca thickness. The conclusion is further supported by the environmental association fusulinid tests: smaller tests or more volutions tend to occur in environments of greater hydrodynamic energy. This study has important implications for hydrodynamic adaptation and metabolism of ancient fusulinids.

Advisor: Dr. S. Xiao

BIOMOLECULAR CONTROLS ON SILICIFICATION PROCESSES

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Biomineralization refers to the biologically mediated or induced organization of solutes to form minerals and amorphous materials. The process of silicification is an important biomineralization strategy used primarily by a variety of unicellular marine organisms to manipulate and build elaborate skeletal parts (figure 1). These elaborate morphologies arise because biogenic amorphous silica (B-SiO_2) is an extremely pliable, and versatile material. It is now believed that the relative abundance of silicifying versus calcifying organisms significantly affects global climate cycles, because their proportion determines the uptake of atmospheric CO_2 by the surface ocean (Van Cappellen, 2003, *RIMG* 54:357-381). In modern oceans, diatoms are the dominant planktonic species, and their activity regulates the abundance of soluble silica to levels that are extremely undersaturated with respect to amorphous silica. Diatoms are also highly effective at sequestering organic matter from surface waters, and account for ~50% of all carbon capture by photosynthesis (Smetacek, 1999, *Protist* 150:25-32).

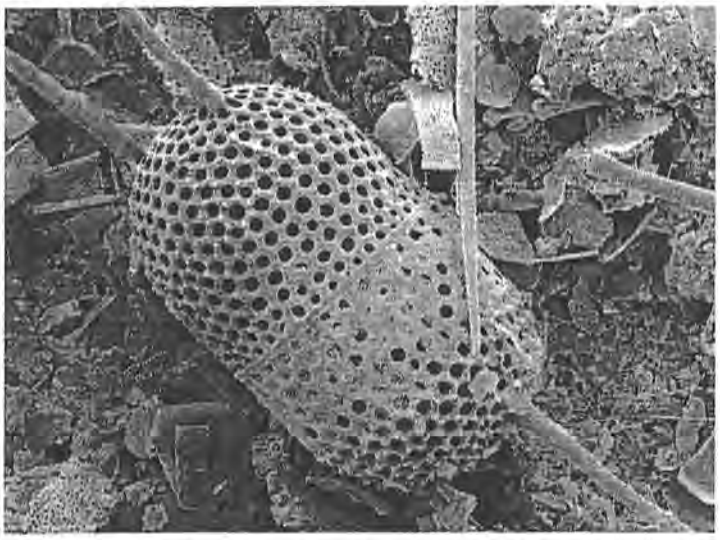

Figure 1: SEM image of a marine Diatom

The biologically mediated formation of amorphous silica requires the importation and storage of high concentrations of soluble Si species. The nature of this reactive silicon pool is unknown, and Si may exist metastably as monosilicic acid, or as stabilized complexes with intracellular components. Recent investigations of amorphous silica nucleation in the presence of cell membrane proteins, polysaccharides, and polyamines in diatoms have shown that certain cell membrane components effectively promote the formation and aggregation of amorphous silica nanospheres (Kröger et al., 1999, *Science* 286:1129-1132). However, these investigations employed complex biomolecules that exhibited multiple functionalities and therefore, it has not been possible to unambiguously resolve which chemical moieties actively promote the formation and agglomeration of B-SiO_2. The first phase of our research will focus on the design of simple experimental and theoretical model systems that will enable us to quantify how specific chemical moieties regulate the thermodynamics and kinetics of amorphous silica nucleation.

The experimental model system will resemble the actual nucleation environment. Metallized <100> surfaces of silicon will provide reproducible, smooth substrates that can be readily coated with a suite of selected compounds that express the desired chemical moieties as a monodisperse surface layer. Interaction of this surface layer with silicic acid will be monitored with *in situ* observational and spectroscopic techniques. This study will advance the understanding of how macromolecules modify the barriers to nucleation, affect growth, and the mechanism(s) by which these processes occur.

Advisor: Dr. P.M. Dove

CHARACTERISTICS OF FLUIDS IN ALKALINE INTRUSIVE ROCKS

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Rocks defined as alkaline are those in which the bulk-rock alkali content exceeds the alkali feldspar molecular ratio [$(Na_2O + K_2O):Al_2O_3:SiO_3$] of 1:1:6, with either Al_2O_3 or SiO_3 being deficient. The excess appears as feldspathoids, sodic pyroxenes, sodic amphiboles and other alkali-rich phases. The alkaline rocks contain a characteristic assemblage of minor and trace elements with significant variation in concentration between massifs. Usually the "alkaline" term is used to encompass a wide range of igneous rocks, not all of which obey the alkali feldspar ratio rule described above. Carbonatites, for example, are certainly silica-deficient but are rarely alkali-rich.

Volumetrically, alkaline rocks account for less than one per cent of all igneous rocks, but the alkaline rocks comprise about half of all igneous rock names because of their mineralogical diversity. Evidence for continental alkaline magmatism can be found as far back as the late Archaean. Alkaline rocks are found on all the continents and on islands in all the oceanic basins. Their occurrences may be classified on the basis of tectonic setting into three categories: continental rift valley magmatism, oceanic and continental intraplate magmatism without clear tectonic control, and alkaline magmatism related to subduction processes.

Evidence suggests that volatile components form a significant part and play an important role in the evolution of the alkaline magmas. Fluid compositions have been provided mostly by fluid inclusion studies and thermodynamic considerations.

Many studies have been made of the fluid inclusions in the numerous alkaline massifs all over the world, but mostly on those in the former Soviet Union. Three major types of inclusions can be found: early silicate-melt inclusions, hydrocarbon-rich gas inclusions and late aqueous brine inclusions. *The melt inclusions* usually show high homogenization temperatures between 800-1250°C. The individual phases in the intergrown masses of the melt inclusions mostly are similar to minerals found in the rock. *Hydrocarbon-rich gas inclusions* were shown in several studies from various alkaline intrusions. The gases are predominantly composed of CH_4 (rarely pure) and other more complex hydrocarbons (up to C_5H_{12}), varying amounts of H, and minor amounts of He, N, CO_2 and/or CO. The genesis of these abiogenic hydrocarbons is explained in two models: (1) a late-magmatic model whereby the hydrocarbons are equilibrium products of volatiles exsolved directly from magmas, and; (2) a post-magmatic, disequilibrium model whereby hydrocarbons are generated via Fischer-Tropsch type reactions at ca. 350°C involving CO_2 and H_2O bearing fluids, linked to redox reactions accompanying hydrothermal alteration. *The aqueous brine inclusions* vary widely, from single-, two- or three phase inclusions containing H_2O-NaCl solution, or multiple phases with more complex ionic composition. The most common components are Na^+, K^+, Ca^{2+}, Mg^{2+}, Cl^-, SO_4^{2-}, and CO_3^{2-}. Homogenization temperatures of brine inclusions extend close to 980°C and salt concentration up to 46 wt% NaCl.

These are the coordinates of alkaline intrusive rocks and characteristics of fluid inclusions which will serve as the starting point for my research project. As a first step we will look at the already known fluid systems in the most studied massifs, try to apply the known methods to some other alkaline massifs on which fluid inclusion studies were not yet applied and try to define if there is a connection between the fluid compositions and the tectonic settings of these alkaline massifs.

Advisor: Dr. R. J. Bodnar

SYNTECTONIC GRANITES AND TRANSPRESSIONAL DEFORMATION AT PEMAQUID POINT, MID-COAST MAINE

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Precision digital mapping and data collection techniques were used to map outcrop structure at several sites along the Pemaquid Point shoreline of midcoast Maine. The regional bedrock consists of tightly folded Bucksport Formation and syn- to post-tectonic granites of the 367 my Waldoboro pluton. Strain partitioning during Late Devonian transpression in a broad area of regional strain accommodation related to the dextral Norumbega shear system allowed for the initial emplacement of granites perpendicular to the L2 hinge parallel stretching lineations within oblique F2 upright folds. Shearing parallel to the oblique fold limbs resulted in rotation, stretching and boudinage of these early orthogonal granites where the sense of local shearing provides constraints on modeling of regional Norumbega deformation.

Asymmetric features in these exposures offer evidence for layer-parallel sinistral shear not dextral as seen in the Casco Bay area closer to the main fault. Counter-clockwise rotation during sinistral shear in the Pemaquid area generated kinematic indicators that include oblique boudin strings, rotated quartz veins and partings, and distortion of quartz fill at boudin necks. Steeply-plunging hook-shaped flanking folds demonstrate layer-parallel sinistral shear around larger boudins.

The distribution of poles to metamorphic layers in stereonet helps to delineate the local SW-plunging F2 fold axes parallel to prominent stretching lineations in the rocks. Post-tectonic quartz veins, granite intrusions and quartz-filled partings during boudinage are perpendicular to these lineations. Earlier variably-deformed veins and intrusions have been rotated to oblique angles to the layering during sinistral shearing. The shear geometry as indicated by the distribution of poles for undeformed to deformed granites is constrained within the metamorphic limb layers with counter-clockwise rotation about a steeply plunging rotation axis. The sinistral antithetic shear observed at Pemaquid Point supports both the *CW fold rotation with antithetic shearing model* [Swanson, 1999] and a new *lateral escape model* for regional strain accommodation. The evidence presented here for sinistral antithetic shear in the Pemaquid area will prove pivotal in refining our understanding of Norumbega-related deformation.

Advisors: Dr. R. D. Law and Dr. M. Swanson

MAGNETIC SUSCEPTIBILITY ANALYSIS OF UPPER MISSISSIPPIAN PALEOSOLS: PALEOCLIMATIC IMPLICATIONS

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Mineral magnetic studies have been applied to almost every aspect of geology. These types of studies can yield information which is similar to other mineralogical techniques (X-ray diffraction or heavy mineral analysis) but often with greater efficiency and resolution. Magnetic susceptibility measurements may be diagnostic of specific processes, like burning, atmospheric pollution or soil water-logging and these types of diagnostic applications are becoming increasingly important to particular areas of study, such as climate reconstruction, archaeology and soil science. Research also has demonstrated the usefulness of magnetic properties as proxy indicators for paleoclimate and sediment mineralogy. To date, extensive research has been done on Quaternary sediments; however, little has been done in terms of ancient siliciclastic sediments. The application of these measurements to ancient systems could provide a valuable new technique to aid in understanding paleoenvironments and their response to climate. Climatic controls on sequence development within terrigenous siliciclastic sediments may be better understood using magnetic susceptibility techniques. Furthermore, this study is designed to develop new procedures that aid in recognizing and defining possible fourth-order sequence boundaries within ancient siliciclastic sediments. These magnetic techniques provide new methods for refining high-resolution sequence stratigraphy in continental successions.

This study focuses on resolving two problems associated with Upper Mississippian Appalachian siliciclastic sediments using magnetic susceptibility techniques. The first problem concerns the ongoing debate between a proposed 'climate' model and a 'rising water table' model in regards to the origin of the green-gray/ grey-white paleosols and coaly zones within the Mauch Chunk Group siliciclastic units. The second problem concerns the use of magnetic susceptibility to determine the location of fourth-order sequence boundaries within these Upper Mississippian siliciclastic units. Since little has been done in terms of magnetic analyses on ancient non-marine sediment, the scope of this study is to develop new techniques that will provide the ground work for future magnetic based research.

Advisor: Dr. K. A. Eriksson

BRINE MIGRATION IN CHADIAN-BRIGANTIAN CARBONATE STRATA OF SOUTHEASTERN IRELAND

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Source and timing of fluids associated with sulfide mineralization in Waulsortian (Courceyan to Chadian) strata of the southern Irish Midlands remains problematic. Prior studies of ore and gangue carbonates in the Rathdowney Trend Zn-Pb district indicate mineralizing fluids that originated from seawater evaporated near and beyond the point of halite precipitation. In this study, Supra-Waulsortian strata were examined from the margin of the Leinster Massif westward to the Rathdowney Trend. Drillcore samples of late diagenetic cements from three localities were examined using cathodoluminescence, fluid inclusion microthermometry, halogen geochemistry, and carbon, oxygen, and strontium isotope geochemistry. Cl/Br ratios of inclusion fluids in these cements indicate evaporated seawater as a likely fluid source. The presence of length-slow chalcedony, quartz, and dolomite pseudomorphs after gypsum and halite in Supra-Waulsortian platform and ramp carbonates in this region indicate evaporative conditions during sedimentation. This also suggests a source for the evaporated seawater fluid involved in mineralization and dolomitization. Regional cathodoluminescence of epigenetic dolomite cements is inconsistent in the studied cores, and does little to help constrain timing of fluids. Fluid inclusion microthermometry and halogen analyses, and isotope data indicate multiple (local) fluid sources and may show that mixing occurred prior to precipitation of cement material. Covariation of strontium isotope values with salinity may indicate the presence of a brine migration from strata proximal to the Leinster Massif to the Rathdowney Trend. The data is consistent with local thermal convection of fluids into Lower Paleozoic basement rocks, and does not support a gravity driven cross-basin flow model.

Advisor: Dr. R. J. Bodnar

EXPERIMENTAL EVOLUTION: EXAMINING FREEZE/THAW CYCLE VIABILITY OF *E. COLI* AFTER 20,000 GENERATIONS

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Most studies in evolution are conducted strictly using a comparative method. This method either examines present-day organismal diversity to infer historical relationships or directly observes paleontological changes through time. Conversely, long-term experimental evolution allows researchers to observe evolution "in action" over many generations. This study examines the dynamics of evolutionary change through 12 populations of *E. coli*, propagated for 20,000 generations at 37C under minimal glucose conditions. Correlated changes in other traits (mutation rates, cell size, gene expression) have been previously associated with the improvement in competitive ability in the selective environment. The main goal of this study is to determine whether the evolved lines changed in their ability to tolerate the stresses of freezing and freeze-thaw cycles.

A population of *E. coli* exposed to freezing and thawing without an added cryoprotective agent (e.g. glycerol) will experience a severe loss of viability. This loss appears to be directly proportional to the number of freeze-thaw cycles. After the bacteria are frozen, the mortality rate only increases if the freezing temperature decreases further. Thus, freezing and thawing seems to cause the cellular damage associated with loss of viability, not the time spent in the freezing state (as long as the freezing temperature does not change).

The average daily mortality rate of the ancestral and evolved strains did not decrease significantly (<3%) at a constant freezing temperature of -80C. This suggests that the time spent frozen was not a major control on mortality. The daily mortality rate increased 34% under a freeze-thaw regime for the ancestral strains, and increased ~50% for the 20K strains. These results emphasize the severe damage freeze/thaw cycles induce on both lines. Recent genetic evidence (from another related study) shows that the adaptation to minimal glucose growth conditions indirectly caused a deleterious mutation that affected tolerance to freeze/thaw cycles. The results of this study may be applicable to the geosciences, including the fields of geomicrobiology, biogeochemistry, and geobiology.

Advisor: Dr. M. F. Hochella, Jr.

LIGAND PROMOTED DISSOLUTION IN SILICATE MINERALS: TRUE OR FALSE?

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Because some minerals show enhanced solubility in the presence of organic complexing agents, there is a widely held idea that these organic ligands cause some minerals to dissolve faster. This "ligand promoted dissolution" rate idea can be correct only if the ligand participates in the activated complex for the dissolution reaction. This means that the effect of organic ligands on the dissolution rate of silicate minerals can be used as a molecular probe of the reaction mechanism. Although ligand promoted dissolution is generally accepted within the geologic community, few studies have documented this phenomenon using silicate minerals. Additionally, no study has produced a rate law that can be used to quantify the effect of ligand concentration on dissolution rate. Many of the studies that have been published contain questionable data derived under less than ideal conditions.

In order to further understand both the reaction rate and reaction mechanism governing ligand-promoted dissolution, I have undertaken a quantitative study of silicate mineral dissolution at varying pHs with varying concentrations of organic ligands. Olivine was chosen as our test mineral because it is one of the few silicates that dissolves congruently, making it a useful model system from which generalizations about all silicate minerals can be made. Because it dissolves more quickly than most silicate minerals, experiments are easier and faster to run than for minerals that dissolve more slowly. Additionally, a rate law for olivine dissolution in acidic solutions has already been established by Rosso and Rimstidt (2000), making comparison between ligand-promoted and ligand-free rates simple.

We expect one of three outcomes to these experiments. The first possibility is that the rate will be enhanced by the presence of the ligands. In this case, we will vary the ligand concentration as well as the pH to try to quantify this effect. The second possibility is that the addition of the complexing agent will have no effect on the dissolution rate. The third possibility is that the addition of the ligand will slow down the dissolution rate by bonding to Mg sites on the surface and blocking them from reacting with H_2O molecules, as they normally would in proton-promoted dissolution. If possible, we will develop rate laws that quantify how varying ligand concentrations affect dissolution rates over a range of pHs. Additionally, we hope to infer a model of the reaction mechanism which drives this reaction.

Dissolution rates will be measured using an internally-stirred, mixed-flow reactor. Samples will be analyzed for magnesium by atomic absorption and for silica by the silicomolybdate blue colorimetric method. The dissolution rate will be calculated by multiplying the concentration of Mg or Si in he effluent by the flow rate of solution through the reactor ($r = r_f m_{mg}$ and $r = r_f m_{si}$).

Advisor: Dr. J. D. Rimstidt

HYDROLOGIC CHARACTERIZATION OF SINKHOLES USING A MULTI-METHOD APPROACH.

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We are conducting a multi-disciplinary study investigating the transport of contaminants from application of waste residuals, such as animal manures and biosolids, within sinkhole environments. As the first step of this larger project, we are utilizing a combination of methods to characterize sinkholes, including electrical resistivity surveys, well drilling, and soil sampling. The electrical resistivity surveys are being conducted to reveal information about subsurface features such as voids, pinnacles, solutionally enlarged joints, and channels that influence groundwater flow and contaminant transport within a sinkhole environment. The characterization data will then be utilized to determine the best locations for installation of wells that will be used to monitor contaminant transport. In addition to aiding in characterization, the electrical resistivity surveys conducted at the same locations during dry periods, and again during wet periods, will allow further characterization of how groundwater moves in a localized sinkhole flow system. Results of this study will have implications for understanding transport of agriculturally-related pollutants in sinkhole systems, and will be used to provide better guidelines for managing waste residuals.

Advisor: Dr. M. E. Schreiber

MICROBIAL ELECTRON TRANSFER MECHANISMS

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Electron transfer reactions are fundamental to the metabolism of microorganisms. They provide us with the fundamental molecular level understanding of the answer as to how microbes breathe minerals. Cellular level mechanistic studies have provided us with the bulk of the present knowledge of these electron transfer mechanism. The two principle mechanisms identified so far are the direct pathways and the relatively new concept of indirect extracellular electron transfer processes. The 'proton motive force' associated with 'membrane bound protein facilitated electron transfer' generates energy for the cell and so most of the present work has focused on the membrane bound or associated molecules, to understand their structure and their mechanisms. As of now the scientific literature has detailed descriptions about the structure and mechanism of electron transfer of various membrane bound proteins, or the direct mechanism. But recent advances in the understanding of electron transfer between microbes and insoluble minerals have focused attention on the possibility of extracellular electron transfer mechanisms involving various small molecules. These mobile molecules are small enough to undergo redox cycling and act as electron shuttles. Much work has to be done to understand the mechanisms and structures of these various small molecules. The study of extracellular electron transfer is still in its infancy and represents a promising area for future research, especially most of the work has to be done in relation to extracellular electron transfer in biofilms.

Advisor: Dr. M. F. Hochella, Jr.

FELSIC MAGMATISM IN FLOOD BASALT PROVINCES: A STUDY OF THE SOUTH MOUNTAIN (CATOCTIN) HIGH SILICA RHYOLITES

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The early Cambrian Catoctin Volcanic Province of the central Appalachians represents a sequence of extension related magmas associated with the opening of the Iapetus Ocean. In the South Mountain region of Pennsylvania and Maryland, the Catoctin Formation is composed of intercalated, sub-aerial rhyolites and basalts. This bimodal association of the volcanic rocks is mostly absent in the rest of the Catoctin Formation rocks further south, which are dominated by basalts. The rhyolites are predominantly glassy lava flows or welded tuffs with feldspar (dominant), quartz, biotite and ilmenite phenocrysts. Preliminary geochemical data identify these rocks as high silica (72-79 wt. %) and low Ti (0.1-0.4 wt %) rhyolites. They are dominantly peralkaline ($Na_2O + K_2O \sim 8$-10%), with A-type affinities. Trace element signatures suggest K-feldspar fractionation as the dominant mechanism of the observed REE patterns. Ba contents can be used to sub-divide the rhyolites into two groups – high Ba (660-840 ppm) and low Ba (<310 ppm). The high-Ba group exhibits elevated Nb, Ta, Ga, Eu, TiO_2, Al_2O_3, and MgO and lower SiO_2 values. The Mount Rogers Formation (750 Ma) rhyolites (types A & B) are similar to the low-Ba Catoctin rhyolites. Petrogenetic models of rhyolites in other continental flood basalt provinces like the Paranás (Brazil), the Karoo Province (Africa) and the Deccan Traps (India) suggest partial melting of underplated mafic rocks near the crust-mantle boundary. The mafic source regions for these rhyolites is supported by distinct trace elemental properties (e.g., ratios for Tb/Yb ~ 0.38, Nb/Ta > 15 and Y/Nb < 1.20). In contrast, rhyolites from South Mountain exhibit an average Nb/Ta ratio (11.1) similar to average crustal values. This crustal signature is also suggested by analysis of Yb/Ta vs. Y/Nb correlations, where the Catoctin rhyolites exhibit measurable differences from OIB-like source field. The understanding of the chemical and temporal evolution of rhyolites in basaltic provinces may provide clues to the development of rifted continental margins.

Advisor: Dr. A. K. Sinha

USING TIME DOMAIN REFLECTOMETRY AND SURFACE ELECTRICAL RESISTIVITY METHODS TO INVESTIGATE THE TEMPORAL AND SPATIAL OCCURRENCE OF GROUNDWATER RECHARGE IN THE BLUE RIDGE PHYSIOGRAPHIC PROVINCE

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Ongoing geophysical investigations at the fractured-rock research site in Floyd County, Virginia suggests that spatial and temporal water-table conditions are useful indicators of where recharge may be occurring in the Blue Ridge Physiographic Province. Surface electrical resistivity profiling at the site has shown that the structure of the regolith (soil and saprolite) is highly heterogeneous, and that localized water table conditions in the regolith can be coincident with underlying vertically oriented faults and fractures that may serve as pathways for preferential flow and ultimately recharge to the crystalline bedrock aquifer.

Preferential recharge zones have been identified through the analysis of surface electrical resistivity data, but little is known about the seasonal variation in recharge rates within these zones, or in the presumably less permeable regolith adjacent to these zones. A more detailed investigation of these recharge processes is underway, which is aimed at providing more detailed measurements of the temporal and spatial variations in soil moisture.

Time domain reflectometry (TDR) profiles collected at weekly intervals at selected locations in the unsaturated zone at the field site are yielding data that support the hypothesis of highly localized recharge zones. Small but perceptible changes in soil moisture content in an area coinciding with a thrust fault shear zone have been recorded with TDR at depths exceeding seven meters, while profiles obtained after the same recharge event in other areas of the site suggest the existence of barriers to deep recharge. High resolution resistivity profile data are being collected to corroborate the vertical TDR profile data.

Continued profiling of these zones will provide information pertaining to the spatial and temporal variation of soil moisture and relative recharge rates in the unsaturated portion of the site. This data set can then be correlated with existing data from continuous water level recorders to establish a link between aquifer response and precipitation events, and will serve as a vital parameter for the calibration of a 2D unsaturated zone recharge model at the fractured–rock research site.

Advisor: Dr. T. J. Burbey

NONLINEAR DYNAMIC SITE RESPONSE FOR EARTHQUAKE HAZARD ANALYSIS IN SOUTH CAROLINA

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Site response due to near surface geologic conditions is an important element in determining the nature of ground motion at any location and is difficult to incorporate in regional scale probabilistic seismic hazard analyses. The purpose of this study is to develop a risk-based, seismic hazard assessment that includes variable site conditions encountered across the state of South Carolina. The results will be used to assess highway bridge design procedures by the South Carolina Department of Transportation (SCDOT). Generalized models for site response analysis involving a variety of near-surface geologic settings in South Carolina are made using predictive equations developed by Andrus et al. (2003). That work is based on cone penetration tests, standard penetration tests and geotechnical laboratory data and predicts strain-dependent material properties and elastic moduli for South Carolina soil conditions. The rock input motions for the site response calculations are derived from a Probabilistic Seismic Hazard Analysis (PSHA) (Chapman, M. C. and Talwani, P. 2002). The subsurface models produced by the predictive equations of Andrus et al. are used for non-linear dynamic site response analysis to produce ground motion estimates appropriate for the study area. The modeling results, in the form of risk-based estimates of response spectra and ground motion acceleration time series, will be compared with the peak acceleration and response spectra currently in use by SCDOT.

Advisor: Dr. M. C. Chapman

THE EFFECT OF SECONDARY PRECIPITATES ON THE DISSOLUTION RATE OF CALCITE IN AMD SOLUTIONS

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Crushed limestone beds are a cost-effective, commonly-employed method used to neutralize the acidity and increase the net alkalinity of acid mine drainage (AMD). However, during this treatment secondary mineral coatings form on the limestone (armoring) slowing its dissolution rate and reducing the effectiveness of this treatment. Anoxic limestone drains (ALD) are used to prevent ferrous iron from oxidizing thereby avoiding the precipitation of ferric iron oxyhydroxide coatings on the limestone surfaces. New investigations indicate that high sulfate concentrations in AMD can lead to the precipitation of gypsum coatings on the surface of dissolving calcite. Experiments that measure the rate for calcite dissolution in conjunction with gypsum and/or iron hydroxide precipitation on the surface of calcite show that under some conditions gypsum rather than iron hydroxide coatings may be the key player in slowing the dissolution rate of the limestone.

The experiments utilize an internally stirred, mixed-flow reactor with calcite as a primary phase on which the formation of secondary phases is induced. The composition of the initial solutions is varied using (1) nitric acid and (2) metal sulfate solutions to simulate the range of pH and [SO_4^{2-}] observed in AMD. The rate (r, mol/m^{2}sec) of dissolution of calcite inhibited by gypsum precipitation on the surface based on H^+ consumption (Fig. 1) and Ca^{2+} release (Fig. 2) measured over time fit power law expressions where dn is the change in the concentration of H^+ or Ca^{2+} (mol) and t is time (sec). These experiments showed that calcite dissolution rates slow with time as the calcite surface becomes coated with secondary phases.

Scanning electron microscopy shows the distribution and type of the coatings on the calcite surface. The rate and coating data from the dissolution experiments provide a basis for a quantitative model and can be used to help understand the general problem of coupled dissolution and precipitation reactions.

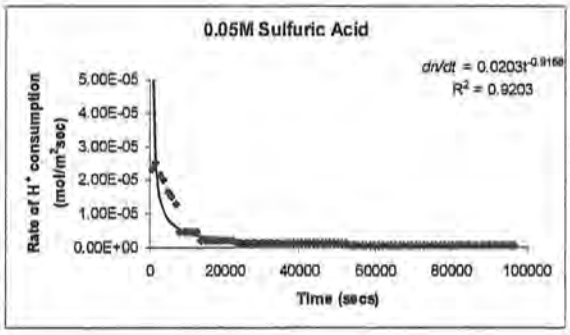

FIGURE 1. Rate of calcite dissolution measured using proton consumption versus time.

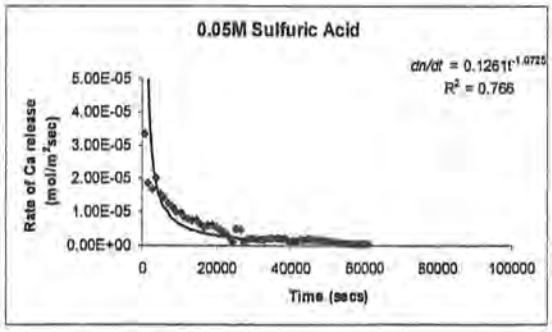

FIGURE 2. Rate of calcite dissolution measured using Ca release versus time.

Advisor: Dr. J. D. Rimstidt

REEQUILIBRATION OF FLUID INCLUSIONS IN TOPAZ

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Microthermometry is one of the most vital techniques when analyzing fluid inclusions but measured homogenization temperatures (T_h) may be higher than the true T_h due to prior heating. This problem is caused by an increase of the internal pressure as temperatures rises, which then produces a volumetric increase. The change in size is not accompanied by loss of the inclusion contents. If an inclusion is heated or pressurized significantly, during metamorphism for example, fluid loss can occur. However, in most cases stretching is more of a problem than cracking due to the difficulty in observing its effects, other than scatter of the T_h.

Reequilibration studies have shown that there is a strong correlation between the hardness of the host mineral and the decrepitation pressure needed to cause deformation of inclusions. Harder minerals, such as quartz, are better hosts than softer minerals, such as calcite or fluorite. However, one important factor that has not been examined is the role of cleavage on reequlibration. Quartz, lacking cleavage, has been analyzed previously (Sterner & Bodnar, 1989) and so an equivalently hard or harder mineral was necessary for this study. Topaz was chosen as it has a hardness of 8 on Mohs scale, has one direction of perfect cleavage, and is a common host of fluid and melt inclusions in igneous rocks.

Synthetic fluid inclusions rather than natural ones are used because we have greater constraints on the composition of the fluid and know exactly what the temperature and pressure conditions were at their genesis. Minor adjustments were made to the standard technique of creating synthetic fluid inclusions in quartz. Individual crystals were collected from the rhyolites present at Topaz Mt., Thomas Range, Utah. They were then examined for the presence of any natural fluid inclusions as only those without fluid inclusions were selected for this study. Doubly-distilled pure water was chosen as the fluid medium because the phase diagram for water is very comprehensive. Samples were placed in cold-seal pressure vessels at 700° C and between 2-3 kbars in order to simulate realistic trapping conditions and also to utilize the stability of topaz. Preliminary results indicate that fluid inclusions were created in large enough quantities for analysis.

Advisor: Dr. R. J. Bodnar

EXTENSIONAL TECTONICS IN COLLISIONAL OROGENS: A CASE STUDY OF EARLY SILURIAN EXTENSION IN THE CENTRAL APPALACHIANS ASSOCIATED WITH THE TACONIC OROGENY

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In many orogens, an extensional event subsequent to a crustal thickening episode has been recognized through both structural and petrologic studies. We describe a similar temporal association in the central Appalachian orogen of Virginia. New ion probe zircon ages of igneous rocks along the axis of collision suggest a 441 Ma igneous event where plutons are identified as suturing tectonic blocks assembled during the collision process, thus marking the end of the compressional phase of the Taconic Orogeny. U/Pb zircon ages (SIMS) of mafic complexes (Rich Acres, Buckingham, Diana Mills and Green Springs) in the same region are well constrained between 434 and 431 Ma, and denote episodic emplacement of mantle derived magmas at mid-crustal levels. These mafic rocks show a range in Mg# (60 to 68), SiO_2 from 46 to 59 wt.% and total alkalis of 2-6 wt.%, and can be classified as gabbro to diorite. High field strength element data (Zr/Hf of 30 to 40; Zr/Nb of 10 to 20; Nb/Ta of 5 to 10) as well as Ba-La-Nb between the plutons are in a narrow range, suggesting a similar source, but different from mid-ocean ridge or ocean island basalts. The strontium isotopic signature (0.7047 to 0.7063) and enriched REE data suggest derivation from either an enriched (metasomatized) mantle and/or a product of crustal contamination. Although no extensional faults of Silurian age have been recognized, we suggest that the sequence of igneous events is most likely to be the result of extension following a mid-Ordovician collisional event. Two tectonic models are permissible (gravitational collapse or slab delamination); however, we propose extension was induced through plate delamination, as gravitational collapse is less likely because of the narrow width of the collision zone. Our data is consistent with a continent-arc collision subsequent to attempted subduction of the passive margin, leading to slab delamination and resultant uplift and extension. In such a tectonic environment hot asthenosphere is likely to intrude the lithospheric mantle of the overriding plate, leading to partial melting. These melts are transported to mid-crustal levels (presumably along structural discontinuities) and are recorded as the mafic plutons in the collision zone.

Advisor: Dr. A. K. Sinha

RELOCATION OF EASTERN TENNESSEE EARTHQUAKES USING HYPODD

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The Eastern Tennessee Seismic Zone is the most seismically active area in the Southern Appalachians. To better understand fault structure and orientation in East Tennessee, the program hypoDD (Waldhauser, 2001) is being applied to 993 earthquakes that occurred between 1984 and 2002. HypoDD uses a double-difference algorithm to minimize the errors due to un-modeled velocity structure.

A total of 120 stations are used to obtain the hypocenter locations. The majority of stations use vertical component, 1 Hz sensors. We use catalog P and S wave arrival times to obtain refined hypocenters. Our preliminary results are based on 550 events with good pair-wise observations forming continuous links. Thirty-six stations recorded P and S wave arrival times from at least 50 events. A minimum of 8 P and S wave observations are used for the double-difference locations, and the average distance between hypocenter pairs is 14 km. We are using the 1D velocity model of Vlahovic et al., (1998).

The hypoDD relocations show changes in small scale hypocenter clusters. Some of these clusters may represent actual fault structure at scales of a few km or less. It appears that a significant number of hypocenters occur on east-west trends for inter-events distances of 5-10 km, particularly in the most active, central portion of the seismic zone.

Advisor: Dr. M. C. Chapman

OCEANS IN THE EARTH: HYDROGEN IN NOMINALLY ANHYDROUS MINERALS

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It has been shown that water can be incorporated within the structures of nominally anhydrous silicates and oxides [Bell D.R. and Rossman G.R., 1992]. Although the concentrations of hydrous components vary widely in structures (commonly in the range of 10's to a few 100 ppm H_2O by weight), such trace amounts of hydrous species can have a disproportionately large effect on the physical, chemical, rheological, and electronic properties of the mineral. The examination of water within nominally anhydrous minerals may also shed light on the recycling of water between the crust and the mantle. This study examines incorporation of hydrogen within the aluminosilicate polymorphs, kyanite, andalusite and sillimanite.

Potential hydrogen bonding sites within the aluminosilicate polymorphs were determined based on an analysis of the Laplacian of the electron density distribution, following the method of Ross et al. (2003). The CRYSTAL98 program [Saunders V.R., Dovesi R., Roetti C., Causa M., Harrison N. M., Orlando R., and Zicovich-Wilson C. M., 1998] was used to generate analytical electron density distributions for kyanite, andalusite and sillimanite, and TOPOND [Gatti C., 1997] was used to locate the (3,-3) critical points. The (3,-3) critical points correspond to regions of nonbonding electron pairs and help pinpoint potential sites of electrophyllic attack by hydrogen. Although (3,-3) critical points are found on all oxygen atoms in the aluminosilicate polymorphs, our results indicate that O1 in andalusite and O2 in sillimanite are prime sites for protonation. These oxygens are solely coordinated to three aluminum atoms and have bond valences of 1.88 v.u. and 1.87 v.u., respectively. The location of the (3,-3) critical points indicate that the potential sites are large enough to accommodate hydrogen and also indicate that the O-H bonds in andalusite and sillimanite are highly directional. In andalusite, the O-H vectors lie within (001) and are approximately parallel to [-1 1 0] and [110], consistent with polarized infrared spectra of andalusite. In sillimanite, the O-H vectors also lie within (001) but are oriented closer to [010]. The location of potential sites for hydrogen in kyanite is less clear. However, the positions of the (3,-3) critical points on O2 and O6, which are bonded to four aluminum atoms, have highly optimized geometries for protonation.

In order to test these predictions, hydrogen was introduced in the structures using the Vienna Ab-initio Simulation Package (VASP) [Kresse G. and Furthuller J., 2003]. The results from these calculations not only determine the location of the hydrogen within the structure, but also provide binding energies for hydrogen in different sites of the structures. Hydrogen within the andalusite structure is energetically favored to bond to O1, but will not bond with any oxygen in sillimanite unless a defect is introduced. Calculations are underway to investigate the effect of defects (such as replacement of Si^{4+} by Al^{3+}) on the incorporation of hydrogen in sillimanite. Introduction of hydrogen into the kyanite structure has thus far not been attempted.

Advisor: Dr. N. L. Ross

ASSESSING THE USEFULNESS OF LITERATURE-DERIVED ESTIMATES OF BODY SIZE

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Trends in body size may be related to a range of evolutionary, paleoecologic and taphonomic questions. Efficient assessment of these trends is therefore important for our understanding of the history of life. Here, we evaluate the bias inherent in the use of size data provided by photographs in monographs.

The observed monographic bias can be assessed with respect to four different end-member outcomes. In the best case, monographs yield unbiased estimates of the central tendency of the sampled population. Alternatively, the monographs may yield biased but predictable ("inaccurate but precise") estimates of size. This is acceptable as long as the bias does not vary across time, space, or taxa. Finally, monograph data would be deemed unacceptable for the reconstruction of size trends if they follow either an "accurate but imprecise" or "inaccurate and imprecise" model (i.e., high imprecision implies very low informative value of monograph estimates).

We targeted several species of Neogene bivalves (n=20) and Ordovician brachiopods (n=10) for which we could acquire, from the same locality, data on both monographic and bulk sample estimates for a given species. For each species, we then compared the central tendencies of the monographic measurements against the central tendencies of the bulk sample. The size bias of monographic specimens was also estimated by its percentile value, relative to the corresponding bulk sample estimates. These two approaches allow us to quantify the magnitude and consistency of the monographic bias and test our data with respect to the four end-member scenarios.

Results suggest that monographic specimens are consistently larger than the average sizes of those from bulk samples for the corresponding species. For brachiopods and bivalves, the majority of monographic specimens are located above the 60^{th} percentile of the corresponding bulk samples. However, the central tendencies of monograph estimates for each species show significant correlations with estimates derived from the corresponding bulk samples. Thus, the data follow the "inaccurate but precise" scenario very well. Just as importantly, the bias appears to be consistent across higher taxa and through time. Thus, monographic data should yield meaningful estimates of body size trends through time.

Advisor: Dr. M. Kowalewski

CRITICAL PVTX PROPERTIES OF AQUEOUS SOLUTIONS

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Fluids play a fundamental role in Earth and planetary environments where they are present as meteoric water, seawater, connate water, metamorphic fluids, hydrothermal or magmatic fluids. Therefore, understanding thermodynamic properties of fluids provides an insight to geochemical processes in igneous, sedimentary and metamorphic systems. The focus of this project is to examine the critical behavior and phase equilibrium properties of complex aqueous solutions with solutes that are the most common in many natural environments (NaCl, KCl, $CaCl_2$). A later part of this research will involve the study of partitioning of elements between immiscible liquid and vapor phases in boiling systems.

Critical PVTX properties in some of the binary subsystems in the H_2O-NaCl-KCl-$CaCl_2$ system have already been studied by previous authors. Experimental data have been published on critical phase relations in the system H_2O-NaCl, in dilute KCl-H_2O solutions, and in H_2O-$CaCl_2$ solutions up to 3 molal concentrations. Up to now no experimental work has been done on the critical properties of more than two component systems, even though these solutions approximate the complexity of natural fluids.

In order to examine these properties we are using the synthetic fluid inclusion technique introduced by Bodnar and Sterner (1987). The method of determining the critical pressures and temperatures involves three steps (Figure 1.): 1) Preparation of fluid inclusions at two different experimental (formation) temperatures and a range of pressures; 2) Determination of the pressure of the boundary between the two-phase and the single phase field based on microthermometrical analysis and petrographic observations. Repeating this process with fluid inclusions trapped at different temperatures defines the critical isochore on the phase diagram; 3) Graphical projection of the critical isochore to the homogenization temperature defines the critical P-T conditions. Once critical PVTX properties are determined for binary systems the next step is to study multicomponent solutions. Samples generated during this phase of the research (with many of them representing fluids trapped in the two phase field) will be used to examine partitioning behavior of elements between the liquid and vapor phases.

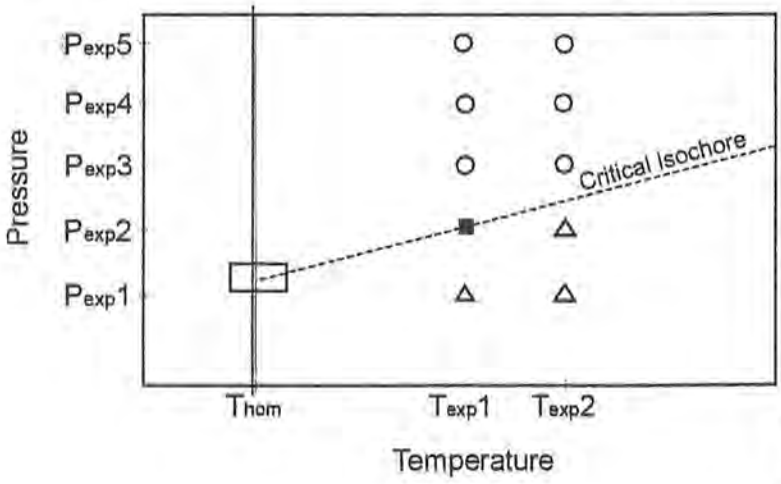

FIGURE 1. Pressure-temperature plot of a critical isochore for sample solution. The box drawn represents the critical pressure and temperature; O, homogenization to liquid phase; △, experiment in the two-phase field; ■, homogenization by critical behavior; T_{hom}, homogenization temperature of inclusions homogenized by critical behavior; T_{exp}, experimental (formation) temperatures; P_{exp}, experimental (formation pressures.

Advisor: Dr. R. J. Bodnar

P WAVE SEISMIC VELOCITY MODEL OF THE SAN ANDREAS FAULT NEAR PARKFIELD, CALIFORNIA

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As a part of EarthScope , the San Andreas Fault Observatory at depth (SAFOD), is a proposed 4-Km-deep drilling project across san andreas fault, near parkfield , California. The aim is to understand the composition, physical state and mechanical behavior of the fault, using insitu data. To assist the planning of the drill hole and interpretation of the data gathered from that, a 50 Km seismic line having 3-component geophone is obtained in Nov 03. The aim is to obtain excellent velocity model and reflection image beneath the drilling site. In the current research the focus is to extend the earlier work (Hole et al, 2001) to obtain the velocity model to a depth of 4-5Km. We will be presenting the preliminary p and s wave velocity model based on refraction traveltime tomography.

Advisor: Dr. J. A. Hole

THERMAL HISTORY OF THE CHESAPEAKE BAY IMPACT CRATER

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The Chesapeake Bay impact crater is a 90 km wide structure that has been described as a complex peak-ring crater; created 35.7 million years ago in the then submerged unconsolidated sediments of the Atlantic coastal plain. An outer rim and annular trough are expressed by the disruption of pre-impact lithologic units. A 38 km inner basin with a peak ring and central uplift is inferred from seismic data. Based on published hydrocode models of the impact there may have been a significant melt sheet and certainly were elevated basement temperatures immediately following the impact in the inner basin. Numerical modeling based on reasonable post-impact temperatures shows heating of syn-impact sediment on the order of hundreds of degrees C for tens of thousands of years after the impact. However, published apatite fission track ages for crystalline basement within the annular trough are consistent with passive margin cooling, indicating maximum impact related temperatures at the top of the basement were under ~110°C at these locations.

Reconstruction of the immediate post-impact thermal history of the Chesapeake Bay impact crater is approached through study of the thermal maturation of dispersed organic matter (DOM) found within syn- and post- impact sediments. More than 60 samples of core from one corehole just outside the crater, two within the annular trough, and one within the inner basin were processed, with about half not yielding enough organic matter for analysis. Two measures of thermal maturity are employed, thermal alteration index (TAI) and vitrinite reflectance.

Results indicate no detectable thermal anomaly associated with syn or post-impact sediments. Mean random vitrinite reflectance (Vm%) values from 16 core samples are between 0.15 and 0.27 % and show no trend with depth or corehole location. These values indicated that the sediments are very organically immature and likely never heated above 30°C for longer then a few tens of years. This is expected for relatively shallow (< 700 meters) Atlantic coastal plain sediments. TAI analysis of 21 core samples yielded a range from 1 to 2+. A TAI of ≤ 2 corresponds to a Vm% ≤ 0.27 and agrees with Vm% data. Three samples were found to have a TAI of 2+, equivalent to an approximant Vm% of 0.5 and a maximum temperature of 80°C. Considering that all four samples had very sparse palynomorphs, that TAI is highly subjective, and that corresponding Vm% values are not elevated, they are not interpreted as an indication of a thermal anomaly.

Thermal modeling is being performed to evaluate varying post-impact temperature profiles and melt sheet geometries, using this maturity data as a constraint.

Advisor: Dr. T. J. Burbey

USING GEOCHEMICAL AND TAPHONOMIC SIGNATURES OF FRESHWATER MUSSEL SHELLS TO EXPLORE INDUSTRY-RELATED EXTIRPATIONS IN THE NORTH FORK HOLSTON RIVER, VA

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The focus of this research is to develop non-invasive techniques to obtain new, independent insights into extirpations (loss of populations) induced by anthropogenic changes. We use freshwater ecosystems of a mercury-polluted river to test the approach. The Olin-Mathieson Chemical Company used mercury to produce chlorine and caustic soda in Saltville, Virginia on the North Fork Holston River from 1950 to 1972. The effluent containing elemental mercury and chloride salts had devastated the freshwater mussel fauna downstream of Saltville by the early 1970's. In a two-pronged approach, we targeted (1) geochemical mercury signatures of empty mussel shells and (2) taphonomic signatures based on quantifying preservational qualities of shells.

The ICPMS analysis shows that shells collected upstream from Saltville (above the pollution source) have very low Hg concentrations (<10 ppb). In contrast, the shells collected directly below the pollution source contain significantly higher Hg concentrations (exceeding 160 ppb for some specimens). Shells collected further downstream have notable Hg concentrations, which decrease with distance from Saltville. Taphonomic signatures of shells also confirm that extirpation patterns relate to the pollution source. Shells are most heavily altered and fragmented in areas directly downstream of the contamination point, which have been devoid of extant populations for at least 30 years, and thus, contain shells that are at least 30 years old. In contrast, upstream sites, unaffected directly by the mercury contamination, contain many fresh-dead shells indicating the presence of reproducing populations, which continuously contribute recent mortalities to the death assemblage. Areas further downstream, which have recently been recolonized by mussel populations, represent an assemblage with an intermediate taphonomic signature.

The study demonstrates that non-invasive techniques focused on dead mussel shells may offer a powerful, independent source of information about freshwater communities with different extirpation and contamination histories. Geochemical and taphonomic signatures of shell remains should become especially useful tools in documenting the pollution history and ecosystem changes in regions with unknown extirpation histories.

Advisor: Dr. M. Kowalewski

UNDERSTANDING TRANSPRESSION FROM PATTERNS OF ROCK UPLIFT ALONG THE SAN ANDREAS FAULT ZONE, CALIFORNIA

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The impact of oblique plate motion on crustal deformation along strike-slip faults is yet to be fully understood. Three existing transpression models for various segments of the San Andreas fault zone make conflicting conclusions regarding the distribution of vertical deformation based on fault strength and obliquity, the angle between the direction of plate motion and the trend of the fault. The wrench tectonic model assumes that fault strength is high and predicts that pure and simple shear will be distributed both adjacent to the fault zone and in the borderlands. In contrast, the stress partitioning model predicts that only simple shear will occur in the fault zone because it is weak, while the convergent component is confined to the borderlands. However, strain partitioning suggests that there is a threshold obliquity angle such that wrenching will dominate at low angles within the fault zone and pure shear will take over at higher angles. Determining the distribution of active rock uplift along the fault zone would therefore isolate the pure shear component of strike-slip faults and create a better understanding of transpression models.

The San Andreas fault zone accommodates oblique convergence along almost half of its length and has well constrained relative plate motion, making it ideal for studying transpressive deformation. To understand the influence of obliquity on rock uplift, bedrock samples from the San Emigdio and northern San Gabriel Mountains along the southern stretch of the fault zone were dated using the apatite radiogenic helium (AHe) technique. The low-temperature sensitivity of AHe dating allows exhumation rates to be constrained for shallow crustal depths and thus provides a valuable measure of recent vertical deformation along the fault. The San Emigdio Mountains represent an ideal setting to test the influence of both high obliquity along the San Andreas fault zone and the intersecting Garlock fault on the distribution of rock uplift. AHe ages indicate that uplift increases southward towards the fault, but other evidence suggests that a possible mismatch exists between geomorphic features and the rock uplift pattern. The northern San Gabriel Mountains are located along a highly oblique section of the San Andreas fault zone with no intersecting faults, so near-field uplift is expected. However, AHe ages indicate that rock uplift can be more rapid in the far field than along the fault zone. In contrast, crustal slivers adjacent to the fault zone at other locations with high obliquity have experienced rapid uplift in the near field, thus following the strain partitioning model. Isolating the differences of rock uplift patterns between the San Emigdio and northern San Gabriel Mountains and other locations along the fault zone is critical for understanding if obliquity plays a primary or secondary role to other factors such as local structure and erosivity in controlling transpressive deformation.

Advisor: Dr. J. A. Spotila

VALIDATION OF UTILIZING ALUMINUM CARBIDE-WATER REACTION TO STUDY WATER-METHANE SYSTEM

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H_2O-CH_4 system can be studied by making synthetic fluid inclusions of various CH_4 concentrations. CH_4 gas can be pumped into the experiment system directly or can be generated during the experiment indirectly by chemical reaction. This study investigates the viability of using an indirect way to making synthetic H_2O-CH_4 inclusions.

When water reacts with Al_4C_3, methane gas will be produced. The reaction equation can be shown as following:

$$12H_2O + Al_4C_3 = 3CH_4 + 4Al(OH)_3$$

Generation of methane has been verified by Raman analysis of the gas phases of the liquid-vapor 2-phase inclusions from the experiments. Presence of the reaction byproduct, $Al(OH)_3$, has been confirmed by X-ray powder diffraction analysis of the reaction residual. By changing the weight ratio of Al_4C_3/H_2O, water-methane systems of different mole concentration of methane can be obtained.

H_2O reacts with Al_4C_3 slowly at room condition, but the reaction rate speeds up significantly with increasing temperature. To secure that the expected molar concentration of CH_4 was generated in the system, a number of calibrating experiments have been done at different temperatures and pressures. The initial findings include:

1. Freshness of Al_4C_3 is a key to the reliability of experiment data. Since Al_4C_3 powder absorbs H_2O in the atmosphere easily and reacts with it slowly, this change in the composition of Al_4C_3, may not be visible, can cause significant deviation of experiment data from the expected ones. Therefore, proper storage of Al_4C_3 is required.
2. When fresh Al_4C_3 was used, the determined CH_4 concentrations in H_2O agree with the expected values satisfactorily, within an error of ±5%, at lower CH_4 concentrations (the expected concentration <4 mol%). However, the discrepancy between the measured CH_4 concentration and the expected CH_4 concentration can be as large as 20%, with an average of 10-15%, when the expected concentration of CH_4 is between 4-10 mol%.

Possible reason for the increased experimental error can be that the reaction rate for H_2O-Al_4C_3 reaction is much higher at higher CH_4 concentration than that at lower CH_4 concentration at the same P-T conditions, so that part of the CH_4 generated and escaped from the system before the system was closed. To verify this conjecture, a technique using glass pipette to protect Al_4C_3 from reacting with H_2O during the sample loading process has been attempted. Experimental error using this technique was lowered in terms of amount of methane produced, but not to a satisfactory degree.

The initial results show that this indirect method to generate CH_4 in H_2O gives reliable data at lower CH_4 concentrations (<4 mol%), when the experiment was conducted appropriately. As for higher CH_4 concentration (4-10 mol%), a correcting equation may be used to calculate the CH_4 concentration in the system in view of the consistency of our experimental data.

Synthetic H_2O-CH_4 inclusions have been trapped at 700C, 2 kilobars successfully . More experiments run at different P-T conditions need to be done in the future. The inclusions trapped under known conditions will be used to determine the phase relationships of H_2O-CH_4 system and is expected to improve the understanding of this important system significantly.

Advisor: Dr. R. Bodnar

MECHANISMS AND KINETICS OF ARSENIC RELEASE FROM IRON OXIDE REDUCTION

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Naturally-occurring arsenic sorbs strongly to mineral surfaces such as Fe(III) oxides. Under aerobic conditions, the Fe(III) oxides are stable, and thus, arsenic remains associated with the solid phase. However, under anaerobic conditions, Fe(III)-reducing microorganisms can couple the reduction of solid phase Fe(III) with the oxidation of organic matter, potentially releasing arsenic to groundwater. Although this process has been documented in a variety of pristine and contaminated environments, minimal information exists on the mechanisms and kinetics of arsenic release.

The objective of this research is to examine arsenic release from Fe(III) oxides due to both abiotic processes (e.g., competition with other oxyanions such as phosphate) and biotic reduction of Fe(III). Arsenic release rates will be determined by conducting controlled experiments using a series of staged batch reactors containing an amorphous arsenic-bearing Fe(III) gel, and an Fe(III)-reducing microorganism, Geobacter metallireducens.

Results of this research will be used to develop mathematical expressions for arsenic release from Fe(III) oxides. These expressions can then be incorporated into other transport models to provide a tool for predicting where and to what extent arsenic is released and transported within anaerobic aquifers.

Advisors: Dr. M. E. Schreiber and Dr. C. J. Tadanier

COMPARISON OF S-WAVE VELOCITY STRUCTURE BENEATH THE KAAPVAAL CRATON FROM SURFACE WAVE INVERSION WITH PREDICTIONS FROM MANTLE XENOLITHS

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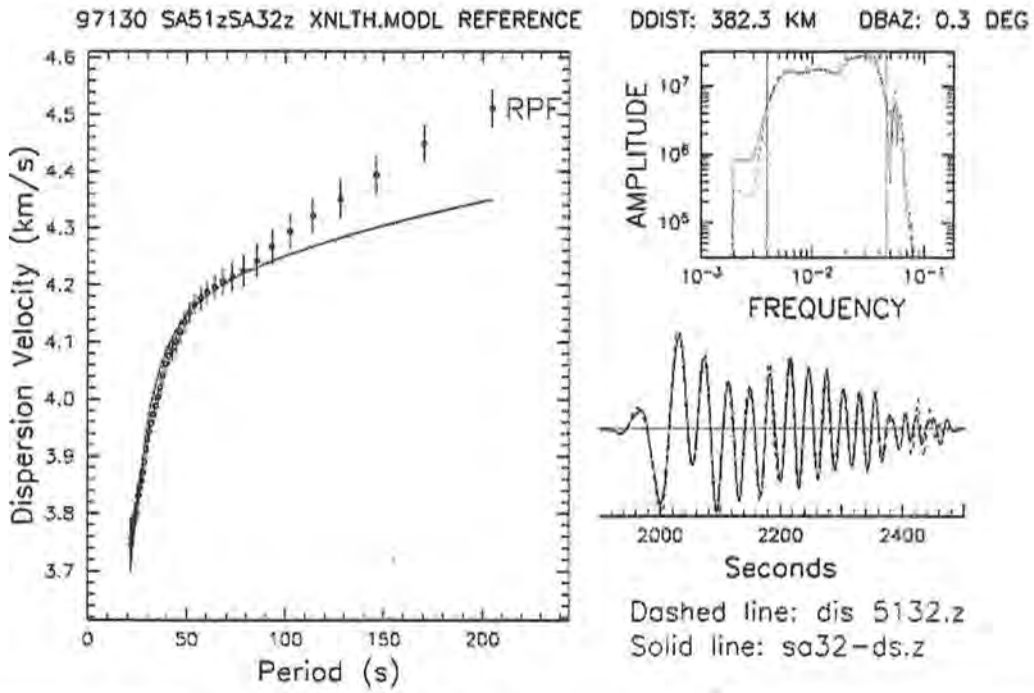
Results from two-station surface-wave inversions across the Kaapvaal craton of southern Africa are compared with seismic velocities estimated from approximately 100 mantle xenoliths brought to the surface in kimberlite pipes. These cratonic xenoliths from the southern Kaapvaal, all less than 100 Ma in age, have been analyzed thermobarometrically to obtain the equilibrium P-T conditions of the cratonic mantle to about 200 km depth. Seismic velocity-depth and density-depth profiles calculated on the basis of these P-T data and the mineral modes of the xenoliths (James *et al.*, *G-cubed*, Jan 2004) are used to produce theoretical surface-wave dispersion curves and to generate starting models for inverting the observed surface-wave dispersion. Preliminary results obtained as part of this study indicate higher velocities present than the predicted velocity-depth curves from xenolith studies at depths greater than 110km. This suggests that a somewhat higher geotherm may have characterized the deep mantle keel at the time of xenolith eruption. A higher geotherm is consistent with evidence that a protracted heating event affected the region in Mesozoic time (Bell *et al.*, *Lithos*, 2003).



The left-hand panel is the interstation phase velocity vs. period plot for the path between SA51 and SA32 for event 97130 located in Iran. The solid line is the predicted phase velocity curve based on the model generated from the xenolith data. The dotted lines in the plots to the right are for spectral amplitudes and the time series from SA51 (near station) projected to the SA32 (far station) epicentral distance using the phase velocities in the left-hand panel. The solid lines are for the (unaltered) SA32 waveform.

Advisor: Dr. J. A. Snoke

KINETICS OF ARSENOPYRITE OXIDATIVE DISSOLUTION BY OXYGEN

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The objective of our study is to use a mixed flow reactor system to determine the dissolution rate and infer potential mechanisms of arsenopyrite (FeAsS) oxidation by dissolved oxygen at 25°C and circumneutral pH. Release rates for iron, arsenic and sulfur are calculated for a variety of initial dissolved oxygen concentrations. Results indicate that the rate of arsenopyrite oxidation, on the order of 10^{-10} mol/m^2/s, is not significantly dependent on dissolved oxygen concentration. Arsenic and sulfur are released in a 1:1 molar ratio while iron is released more slowly due to precipitation either on the mineral surface or within the reactor system. The percentage of As(V) released increases over time; arsenic species may be accumulating and oxidizing on the surface before they are released to solution. These lines of evidence suggest that the rate determining step in arsenopyrite oxidation is reflected by the rate of bond breaking at the anodic site in the mineral, and not the transfer of electrons from the cathodic site to oxygen, as is suggested to be the case for other sulfide minerals such as pyrite.

Previous work on arsenopyrite (FeAsS) oxidation has been limited to low pH conditions with ferric iron as the oxidant. However, not all arsenopyrite weathering occurs exclusively in acidic environments. For example, at our field site at an abandoned arsenopyrite mine in Virginia, the pH of ground and surface waters is consistently between 5 and 7. Results of this study provide important insight to arsenic mobilization processes and rates, at field-relevant conditions, consequently aiding in the effort to understand arsenic release and retention in the environment.

Advisor: Dr. M. E. Schreiber

TIME AVERAGING ON A SHALLOW SUBTROPICAL SHELF

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Studies of rates of time averaging in present-day settings are important for understanding the temporal resolution of the fossil record. The taphonomy of shells has been used in paleontological research as a proxy for time averaging and the duration of pre-burial taphonomic history (age-since-death) with varying results. Here, we use rates of time averaging estimated from directly dated specimens of the tellinid bivalve Semele casali and the terebratulid brachiopod Bouchardia rosea to analyze the informative value of taphonomic signatures on pre-burial history.

The two studied organisms were collected along a transect from two shallow (10 and 30 m) nearshore localities from Ubatuba Bay located on the inner part of the Southeast Brazilian Bight (SW Atlantic), a mixed carbonate-siliciclastic shelf. The two targeted species are approximately the same in terms of size, but differ in many respects. M. cleryana has an aragonitic shell and a shallow infaunal life habit, whereas B. rosea is calcitic and an epifaunal, free-lying suspension feeder. To quantify specimens in terms of preservation, additive taphonomic scores for the presence or absence of disarticulation, fragmentation, edge completeness, glossiness, interior and exterior surface alteration, visibility of muscle scars and shell color were computed. A higher taphonomic score indicates that a shell is more degraded. Ages of shells were estimated using amino acid (D/L aspartic acid) racemization, calibrated against paired AMS-radiocarbon analyses. Taphonomic scores were compared against shell age both between taxa and between collection sites.

Previous studies have indicated that due to shell microstructure, brachiopods may disarticulate and disintegrate faster than bivalves. Data suggest however, that brachiopods in this assemblage (median age 695.7 years) are slightly older than bivalves (median age 250.9 years). Taphonomic scores were also generally greater for brachiopods than for bivalves, and greater at the 30 m site than at the 10 m site. Furthermore, the data agree with previous studies that taphonomic grade of individual shells can not be used alone as a proxy for the duration of its pre-burial history. The use of taphonomy is more promising at the assemblage level, and the level of taphonomic degradation, or taphonomic score of the assemblage does appear to increase with age since death.

Advisor: Dr. M. Kowalewski

TESTING THE ROLES OF CLIMATE, TECTONICS, AND BEDROCK LITHOLOGY IN THE LATE CENOZOIC INCISION HISTORY OF THE NEW RIVER

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The New River is the only major river that drains to the Gulf of Mexico while cutting through three physiogeologic provinces of the Appalachians. In the Virginia Valley and Ridge, the New River has developed a sequence of unpaired fill-cut and strath terraces where it passes from erodible carbonates to resistant siliciclastics. The few dated deposits along this reach of the river (e.g. Granger et al., 1997) indicate a major period of aggradation followed by one or more periods of downcutting, possibly as a reaction to climate change or regional drainage reorganization. Cosmogenic 10Be exposure dating of several terrace levels allows preliminary reconstruction of the New River's incision history, which can be compared to climate events in eastern North America. Mapping of fluvial terraces and related bedrock straths and logging of two cores through 40 m of fill provide a framework for interpreting these ages. Preliminary results indicate a slowing of the New River's incision rate from approximately 120 m/Myr between 0.6 Ma and 0.3 Ma to about 28 m/Myr between 0.3 Ma and the present. The more rapid rate may be related to the evacuation of over 100 m of alluvial fill from which the upper terraces in the study area are cut. The slower modern rate is related to the erodibility of resistant lithologies that outcrop in bedrock-floored reaches of the river. Comparison of soil weathering indices with cosmogenic ages allows further interpretation of incision history based on prior soil chronosequences (e.g. Mills and Wagner, 1985). Cosmogenic exposure ages obtained from higher fill-cut terraces imply that these surfaces are about half as old as previously suggested based on soil development. Young cosmogenic ages could be an artifact of erosion from dated surfaces, especially on older, higher terraces. However, soil profiling suggests that erosion from these surfaces is not extreme, so the cosmogenic ages are regarded as reasonable minimums. Downstream differences in terrace configuration suggest differential incision. Dating of similar surfaces in different reaches of the river and examination of active erosion features on resistant bedrock will help to clarify whether these differences in the New River's incision pattern may be due to tectonic tilting or are due simply to lithologic controls on erosion and deposition.

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SEISMIC RESERVOIR CHARACTERIZATION IN COALINGA FIELD

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Reservoir characterization is a prerequisite for oil field development. The current state-of-the-art is volume visualization and geobody analysis. The major drawbacks are lithologic ambiguities, and yet too much detail for direct use in reservoir modeling. In this project, we drive these approaches to their limit and investigate how to overcome these problems.

Our study focuses on the stratigraphy, lithology and geologic process of the clastic Temblor (Miocene) reservoir in Coalinga, California. The field is close to the San Andreas Fault and contains four unconformable surfaces representing incised-fill to sub-tidal depositional environments, which render the reservoir highly heterogeneous. In addition, cementation often masks lithological signatures on seismic. Coalinga field has produced heavy oil since 1887 and is presently under tertiary development. Current production methods include steaming which results in a tremendous well density. The objective of this investigation is to integrate seismic data, well data, and geologic concepts into developing models with geologic and stratigraphic constraints, internal consistency, and compatibility with seismic data and wireline logs.

We developed a new poststack interpretive static correction technique to map these unconformities on 3D seismic. Advanced computing powers enable us to stretch the resolution limit to the maximum possible with the help of the new technology 'Geovolume Visualization and Interpretation (GVI)'. It provides a method for geoscientists to quickly evaluate complex structural, stratigraphic, and amplitude features in 3D space and helps us to demarcate and delineate the reservoir into sub-units, based on its depositional signatures and geological characteristics. The technology and philosophy of GVI differs dramatically from conventional line-based interpretation and includes new interpretation strategies and methodologies. It incorporates the techniques such as, recognition, color, motion, and isolation. Recognition helps in distinguishing characteristics of an event to be mapped and is followed by further processing to enhance those recognized characteristics for visualization and geobody mapping. With an appropriate color scheme, the resultant color attribute is a direct representation of the seismic attribute distribution. Depth cueing, lighting, and intensity are some of the important components associated with the color viewing. Motion provides the ability to move an object in a manner continuous to the human eye simultaneous with control movements, which allows us in observing how the data is related in space and time. Isolation, the ability to separate events of interest from other data is achieved by rendering the opacity values for the extraneous attribute amplitude values and creating a relatively transparency scheme for marginally important amplitudes. It helps in illuminating stratigraphic and geomorphic architecture within the reservoir.

Our approaches help to demarcate and delineate the reservoir into seismostratigraphic and seismogeomorphic elements bounded by unconformities and depositional geobodies, which in turn, would be able to demonstrate various lithological signatures on 3D-seismic data, constrained and validated by wireline data. We assemble all this data into one deterministic, high-resolution reservoir model. The final result will be a compartmentalized reservoir model of the highest-possible resolution to demonstrate the deterministic limit and serve as benchmark for other reservoir characterization and modeling techniques. Our study is supported by the DOE contract DE-FC26-00BC15301.

Advisor: Dr. M. G. Imhof

STRAIN SYMMETRY AT THE BASE OF THE MOINE NAPPE, NW SCOTLAND: IMPLICATIONS FOR MATERIAL FLOW ALONG OROGENIC STRIKE

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Geometric analyses of thrust systems commonly assume strain is essentially two-dimensional (plane strain--no movement of material across the transport plane). Some early studies have argued that strain accumulation in orogenic belts is characterized by gently dipping L-S tectonites (Flinn, 1956), in which the linear element of the grain shape fabric indicates transport direction. These L-S tectonites could be interpreted as an indication of two-dimensional (plane strain) deformation. More recent studies argue that plane strain may be the "exception rather than the rule" in thrust belts. Many field studies have demonstrated that plastically deformed rocks in an orogenic belt are not simple L-S tectonites, but instead display a range of grain shape fabrics from pure S through L-S to pure L tectonites. At a more fundamental level, formation of L and S tectonites creates major space problems--L tectonites indicate contraction parallel to orogenic strike and, conversely, S tectonites indicate elongation parallel to orogenic strike.

Two approaches have been taken to explain the presence of plastically deformed rocks that vary between L and S tectonites in orogenic belts. These approaches differ in whether the observed grain shape fabrics reflect an apparent or true strain, and on whether these tectonic strains are primarily two-dimensional or are actually three-dimensional (general strain) in nature. However, in plastically deformed quartz-rich rocks, the observed geometric relationships between finite strain axes and the crystal fabrics developed during deformation may be used to define the actual strain path followed by the rock. The combined techniques provide an independent test for determining whether natural strain data indicates true or apparent along-strike stretching. Experimental studies (involving both dislocation creep and dynamic recrystallization), numerical simulations, and analyses of naturally-deformed quartz-rich rocks have consistently demonstrated a simple relationship between strain symmetry and the developed pattern of quartz c- and a-axis fabrics. As strain increases, the fabric pattern strengthens rather than changes.

In the earlier phases of this project, flattening strains have been measured from three-dimensional strain analysis of rocks from Loch Eriboll and Stac Glencoul. Various techniques of quantitative vorticity were then applied to these samples. These data indicate 53-67% vertical shortening perpendicular to the flow plane and 20-50% extension along orogenic strike. In conditions of strict simple shear, neither of these stretches would be possible (c.f. card deck analogy). The vorticity results have generally shown pure shear contributions of approximately 30-57%. It is the presence of a pure shear component that allows for the possibility of actual extrusion along the flow plane (both parallel and perpendicular to the transport direction).

If the general strains indicated by deformed grain shapes are confirmed by crystal fabrics, then this strongly indicates that previously published numerical models for emplacement and internal straining of thrust sheets will need to be modified to take into account the strain compatibility problems indicated by our data. Any along-strike flow of material must be accommodated by development of structures such as folds and faults subparallel to thrust transport direction or by grain-scale deformation processes such as pressure solution. The field area was chosen because much of the research has been concentrated in the Caledonides. The Moine thrust zone was chosen because it contains both suitable strain markers and crystal fabrics, which can be used to determine whether measured strains are true or apparent.

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SHOCK REEQUILIBRATION OF FLUID INCLUSIONS

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While fluid inclusions in terrestrial rocks are nearly ubiquitous, only a few fluid inclusion-bearing meteorites have been documented. The scarcity of fluid inclusions in meteoritic materials may be a result of (a) the absence of fluids when the mineral was formed on the meteorite parent body or (b) the destruction of fluid inclusions originally contained in meteoritic materials by subsequent shock metamorphism. By examining the effects of shock deformation on fluid inclusion properties and textures we may be able to better constrain the pressure-temperature path experienced by terrestrial and meteoritic shocked materials and also gain a clearer understanding of why fluid inclusions are rarely found in meteorite samples. Impact-related fluid inclusion reequilibration has been examined by measuring the properties of fluid inclusions in single crystal quartz disks before and after the samples were subjected to shock waves of well controlled amplitude. Naturally shocked crystalline basement rocks from the Ries Crater, Germany and Meteor Crater, Arizona are also currently being studied to determine whether pre-impact fluid inclusions have experienced reequilibration as a result of natural shock metamorphism.

The experimental results demonstrate that fluid inclusions undergo a systematic and gradual evolution in reequilibration effects with increasing shock pressures. Fluid inclusions initially undergo a decrease in volume (collapse) immediately following impact as the shock wave moves through the sample, producing a relatively high pressure external environment compared to the lower pressure in the inclusion. If the fluid inclusions survive this event intact, the initial volume decrease is overprinted by stretching due to internal overpressures experienced during sustained high temperature conditions as the decompressed rocks cool following the shock event. This portion of the P-T cycle leads to an increase in inclusion volume and homogenization temperature and, possibly, decrepitation. This systematic progression of shock reequilibration features observed in the experimental impact studies may be used to estimate syn- and post-impact pressure-temperature conditions experienced by shocked materials, especially at low pressures that are otherwise difficult to resolve optically. These results also indicate that the absence of fluid inclusions in meteoritic materials does not preclude the presence of fluids on meteorite parent bodies-- instead all previously trapped fluid inclusions may have been destroyed by relatively modest shock processes. Preliminary study of shock metamorphosed crystalline basement rocks from the Ries Impact Crater indicates similar reequilibration effects also occur in naturally impacted materials.

Advisor: R. J. Bodnar

TESTING GEOCHEMICAL REACTIVITY AS A FUNCTION OF MINERAL SIZE: MANGANESE OXIDATION PROMOTED BY HEMATITE NANOPARTICLES

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The rate of Mn^{2+}(aq) oxidation on hematite surfaces in the presence of oxygenated water has been studied as a function of the hematite particles size, where the particles are in the nanometer size regime. Experimental results from this study suggest that the surface area normalized initial heterogeneous manganese oxidation rate is approximately one and a half orders of magnitude greater on hematite particles with an average diameter and thickness of 7.3 nm and 1.5 nm than those with average dimensions of 37 nm by 8 nm. The properties of nanoscale hematite, including the electronic structure and surface chemistry, are expected to change significantly with particle size. The acceleration of electron transfer rate for the reactions promoted by the smallest particles was rationalized in the framework of electron transfer theory, considering the affect of the surface geometric and electronic structure on the electronic coupling, the reorganization energy, and the redox potential of the Mn.

Advisor: Dr. M. F. Hochella, Jr.

QUANTIFYING GEOGRAPHIC VARIABILITY OF A LINEAGE; THE GEOMETRIC MORPHOSPACE OF MULINIA.

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Mulinia has been a ubiquitous mactrid bivalve within the Atlantic Coastal Plain since the Pliocene. Qualitative observations suggest there is geographic morphological variability in both past and present populations. However there are no cited attempts to quantify the degree of geographic variability and determine if the magnitude remains constant within a lineage. This study aims to quantify the variability seen within populations of *Mulinia congesta* and its likely descendant *Mulinia lateralis*. Specimens were used from bulk research and museum collections from Virginia to Florida. *M. congesta* specimens were sampled from Pliocene formations co-eval temporally to the Yorktown Formation. *M. lateralis* specimens were sampled from Pleistocene formations co-eval temporally to the James City Formation and Flanner Beach Formation.

Each valve was digitally imaged and x-y coordinates for fifteen landmarks and pseudolandmarks were acquired. Procrustes method was used to simultaneously fit the landmark points and derive shape coordinates that are invariant in respect to variations in size, rotation, and position of specimens. Tangent coordinates were used to derive principle component ordination to compare the overall shape differences between shells from different regions, and size was estimated using shell length and centroid size.

Preliminary results based on 789 specimens of *M. congesta* from 16 localities suggest that geographic morphospace varies significantly and there is a latitudinal trend based on the amount of specimens misclassified during a jackknife crossvalidation. For specimens originally from Virginia, 9% of them were misplaced into North Carolina, while none were misclassified with specimens from Florida. For Florida specimens, 8.33% were misclassified as Georgia, while 2% were misclassified as Virginia specimens. The amount of variation between geographic regions is comparable to the amount interspecific variation between the two *Mulinia* species, when 68 *M. laterialis* specimens were analyzed. The geographic variability in morphology of *Mulinia* exceeds notably environmental variability and may be comparable in level to interspecific variability within the genus. Geographic gradients may thus exert influence on morphology that is comparable to morphological effects of speciation.

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FRACTURE ILLUMINATION VIA WEIGHTED RADON TRANSFORM

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In principle, the Radon transform has the ability to sum events exhibiting a linear, hyperbolic, or parabolic trajectory in the space-time domain to a single event in the transformed domain. Because of this, Radon filtering has had resounding success in suppressing multiple reflections from normal moveout corrected seismic data.

Subsurface fractures are modeled as local scatterers embedded in a uniform medium. These scatterers produce a hyperbolic coda of wavelets when subjected to numerical models of wave propagation. The apex of these hyperbolas coincide with the location of the scatterer. In order to accentuate these fracture signatures, primary and multiple reflections need to be removed. Primary and multiple reflections produce a "Radon recognizable" hyperbola, meaning their apex occurs at near zero offsets on common shot gather data. These events are focused to a localized event in the Radon domain. On the other hand, the energy associated with the scatterers is "smeared" in the transformed domain. This allows for filters to be designed in the Radon domain that remove much of the energy associated with the scatterers, thus successfully modeling the primary and multiple reflections upon inverse transformation to the offset domain. The modeled primaries and multiples are then adaptively subtracted from the original data to illuminate the fracture signatures.

Advisor: Dr. M. G. Imhof

PETROLOGY OF GARNET-BEARING GRANULITES OF THE VIRGINIA BLUE RIDGE TERRANE

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The Blue Ridge terrane of central Virginia is made up of high-grade gneisses and intruded charnockitic granitoids of middle-Proterozoic age. Relatively pristine granulite-facies metamorphic assemblages are preserved in the rocks of the western Blue Ridge. The gneisses are dominantly medium-grained K-feldspar (Kfs), plagioclase (Pl), quartz (Qtz) and orthopyroxene (Opx) rocks that are weakly to strongly foliated and display a granoblastic texture. The charnockitic intrusives contain similar mineral assemblages, but have a much coarser grain size and are generally massive or weakly foliated. The orthopyroxene in many of these intrusives displays exsolution lamellae of clinopyroxene, suggesting inversion from higher temperature pigeonite. In addition to the minerals mentioned above, some of these rocks also contain garnet (Grt). These garnet-bearing rocks also commonly contain biotite and, in some cases, minor amphibole. Garnet occurs in two forms: 1) as poikiloblastic porphyroblasts and 2) as symplectites with quartz that rim orthopyroxenes and biotites.

The presence of these mineral assemblages allows for the investigation of the evolution of granulite P-T conditions in the Blue Ridge. Many common geothermometers use Fe-Mg exchange reactions between phases such as orthopyroxene, garnet, and biotite. However, these thermometers commonly yield underestimates of P-T conditions because they are easily reset upon cooling of the rocks from their original peak metamorphic conditions. Pattison et al. (2003) have demonstrated that temperatures determined for many of the well-known granulite terranes are likely underestimates by at least 100°C. Their higher temperatures are based on applying an orthopyroxene-garnet thermometer that uses Al-solubility in orthopyroxene and corrects for late-stage resetting of Fe-Mg to the mineral assemblage Grt-Opx-Pl-Qtz. This assemblage is present in many of the Blue Ridge granulites, and thus allows for the application of this thermometer. Temperature estimates of the Blue Ridge based on 2-pyroxene thermometry are in excess of 900°C. Application of the Pattison et al. (2003) thermometer will allow for comparison with this and other geothermometers and also allow for the comparison of the Blue Ridge terrane with other granulite terranes. Applying this thermometer to assemblages containing the two different morphologies of garnet may yield information about portions of the P-T-t path and the tectonic evolution of the Blue Ridge.

Figure 1. Back-scattered electron image of symplectic garnet and quartz around biotite and some orthopyroxene (upper right). Note some symplectic biotite near the top of the image. Scale bar at lower left is approximately 300 μm.

Advisor: Dr. R. J. Tracy