UNIVERSITY OF WYOMING

GRADUATE RESEARCH SYMPOSIUM

Showcasing Graduate Student Achievements in Energy Research

Thursday, April 22, 2010

9:00 am to 5:00 pm

Wyoming Union Yellowstone Ballroom

SCHOOL OF ENERGY RESOURCES

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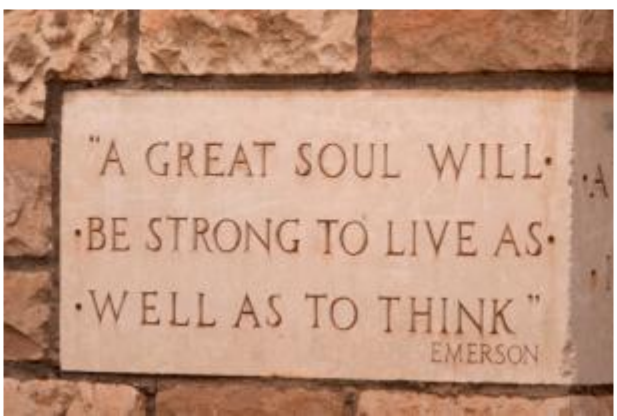
2010 Graduate Research Symposium

April 22, 2010

Wyoming Union
Yellowstone Center Ballroom and Senate Chambers

Agenda

9:00 am – 9:05 am	**Dr. Don Roth** **SER Associate Director for Academics**
9:05 am – 10:00 am	**Poster Presentations, Senate Chambers**
9:05 am – noon	**Oral Presentations, Center Ballroom**
Noon - 1:00 pm	**Lunch (on own)**
1:00 pm - 3:40 pm	**Oral Presentations, Center Ballroom**
4:00 pm – 5:00 pm	**Poster Presentations, Center Ballroom**



The Graduate Research Symposium

provides a forum to showcase University of Wyoming graduate student achievements in energy research and to foster interaction among graduate students in diverse disciplines. It also provides an opportunity for students to enhance their presentation skills for a broader audience and to build their resumes.

2010 Graduate Research Symposium
Thursday, April 22, 2010
Oral Presentations

Time	Yellowstone Center Ballroom
9:05-9:25 am	Corin Chepko Physics
9:25-9:40 am	Open
9:40-10:00 am	Joo Seob Lee Chemical & Petroleum Engineering
10:00-10:20 am	Mehmoosh Moradi Bidhendi Chemical & Petroleum Engineering
10:20-10:40 am	V K C Pakala Mechanical Engineering
10:40-11:00 am	Sarah Ramsey-Walters Science & Math Teaching Center
11:00-11:20 am	William Schaffers Chemical & Petroleum Engineering
11:20-11:40 am	Qing Zhang Civil & Architectural Engineering
11:40-noon	Dawei Mu Geology & Geophysics
Noon-1:00 pm	*Lunch on your own*
1:00-1:20 pm	Jessica Frint College of Law
1:20-1:40 pm	He Huang Computer Science
1:40-2:00 pm	Hee Joon Park Chemical & Petroleum Engineering
2:00-2:20 pm	Xiuyu Wang Chemical & Petroleum Engineering
2:20-2:40 pm	Gevorg Sargsyan Chemistry
2:40-3:00 pm	Michael Stoellinger Mathematics
3:00-3:20 pm	Thomas Sturtevant Atmospheric Science
3:20-3:40 pm	Saeed Ovaysi Chemical & Petroleum Engineering

Graduate Research Symposium 2010
Thursday, April 22, 2010
Poster Presentations

Poster Number	Senate Chambers Presentations 9:05-10:00 am
1	Curtis Chopping Geology & Geophysics
2	Brian Gruver Chemistry
3	Liyou Lu Physics & Astronomy
4	Yitong Luo Civil & Architectural Engineering
5	Amber Mason Renewable Resources

Poster Number	Yellowstone Center Ballroom Presentations 4:00-5:00 pm
1	Daejin Choi Chemistry
2	Cally Driessen Renewable Resources
3	Ping Guo Computer Science
4	Benjamin Kinney College of Law
5	Xiaojing Wang Chemical & Petroleum Engineering
6	Steven Hansen and Amit Padhi Geology & Geophysics
7	Arash Aghaei Chemical & Petroleum Engineering

Arash Aghaei, Ph.D. Candidate
Department of Chemical and Petroleum Engineering
Advisor: Dr. Mohammad Piri
Poster Presentation

DYNAMIC PORE-LEVEL NETWORK MODELING OF MULTIPHASE FLOW IN MIXED-WET CORES

We present a dynamic pore-scale network model that runs on multiple CPUs, and can model two-phase flow processes in core-size networks. Our goal is to develop a model that can predict transport properties of two-phase flow quantitatively which can be compared with results from Special Core Analysis experiments. Some of the applications of these transport properties are in reservoir scale simulations of Enhance Oil Recovery and CO_2 Sequestration schemes. Networks of capillary elements generated from, for instance, high-resolution microtomography images will be used in this work. A core-size network representing a real rock sample has hundreds of millions of capillary elements. Thus we are taking advantage of parallel computing to run our dynamic pore-level model in these large networks. A large network is first decomposed in three dimensions forming a number of blocks. Each block is then assigned to a CPU that does the calculations required for the elements of its own block. Message Passing Interface (MPI) is used to communicate calculation results between CPUs. In order to develop scalable parallel algorithms and achieve maximum performance we minimize latency for all parts of our model. At the core scale, viscous and gravitational forces may become comparable with capillary force, so they cannot be ignored in the model. By taking into account viscous and gravitational forces as well as capillary force, we will be able to study the effects of Capillary number and Bond number on different transport properties. And we will also be able to simulate unsteady-state and steady-state relative permeability experiments.

M. Moradi Bidhendi
Department of Chemical and Petroleum Engineering
Advisor: Dr. Vladimir Alvarado
Oral Presentation

EFFECT OF SALINITY ON WATER-IN-CRUDE OIL EMULSION: EVALUATION OF DROP-SIZE DISTRIBUTION PROXY

M. Moradi Bidhendi and Vladimir Alvarado

The drop size distribution of water-in-oil emulsions prepared with a crude oil from Wyoming using a synthetic brine that mimics a reservoir brine from a Wyoming reservoir at the different ionic strengths have been measured. The drop-size distributions were determined with the objective to determine emulsion stability as a function of brine salinity by tracking changes in the size distributions as a function of time. A procedure for obtaining relatively homogeneous samples of the initial emulsion was developed in such a way that replicas of the initial sample allowed us to measure size distribution through direct observation in an optical microscope. The results indicate that emulsions become more stable as the ionic strength of the brine decreases. This result is consistent with pressure drop increase in low-salinity waterflooding for enhanced-oil recovery purposes.

Corin Chepko, Ph.D. Candidate
Department of Physics and Astronomy
Advisor: Dr. Jinke Tang
Oral Presentation

PREPARING AND TESTING BISMUTH-TELLURIDE BASED THERMOELECTRIC MATERIALS

Corin Chepko and Jinke Tang

Wasted energy, in the form of heat, is produced by many devices, such as in automobiles and computers. Thermoelectric materials can provide a way to recycle a portion of that energy back into electrical energy, thereby increasing the efficiency. A thermoelectric material is characterized by its ZT value, which is an indication of the efficiency of energy conversion. ZT can be improved by increasing the electrical conductivity while decreasing the thermal conductivity of the material. For temperatures around 400°C, Bismuth-Telluride is a widely used thermoelectric material, and with a ZT factor of about 1, bismuth - telluride has a conversion efficiency of 3-4%. The goal of my research is to use a process of mechanical alloying and cold-pressing to reproduce the accepted results for bismuth-telluride, then to try adding various other elements that, according to previous research and theoretical predictions, will improve the thermoelectric properties. The bismuth-telluride produced consists of nano-sized particles, which should improve the ZT value by scattering phonons while still allowing good electrical flow. Different dopants should also improve ZT by scattering more phonons without affecting electrical conductivity. The process of preparing the samples will be discussed as well as some of the results and future work

DaeJin Choi, Ph.D. Candidate
Department of Chemistry
Advisor: Dr. Bruce Parkinson
Poster Presentation

DYE SENSITIZATION OF HIGH SURFACE AREA GALLIUM PHOSPHIDE PHOTOELECTRODES

Gallium Phosphide (GaP) is an interesting material for studying the fundamental process in Dye Sensitized Solar Cells (DSSC) due to its band gap energy, high carrier mobility and proper band position for electron injection from dye excited states. Early work showed that GaP could be sensitized to sub–band gap illumination, however yields were low due to the single layer of adsorbed dye. In this contribution, we investigate dye sensitization, with Rhodamine B and Crystal Violet, of high surface area n-type GaP produced by photoassisted anodic etching of a GaP single crystal. The higher surface area electrodes showed higher sensitization yields. The surface condition of the n-GaP electrode was found to be important for high sensitized Incident Photon to Current Efficiency (IPCE) values. XPS and Mott-Schottky plots were used to characterize the surface oxides before and after chemical, electrochemical and photochemical etching. The presence of the surface oxides usually reduced the IPCE.

Curtis Chopping, M.S. Candidate
Department of Geology and Geophysics
Advisor: Dr. John Kaszuba
Poster Presentation

EXPERIMENTAL APPROACH TO GEOLOGIC CO-SEQUESTRATION

Curtis Chopping and John Kaszuba

Capture and storage of CO_2 in geologic formations (geologic sequestration) is currently one of the most promising technologies for reducing or mitigating anthropogenic CO_2 emissions. In Wyoming, emissions from coal fired power plants contain sulfur, therefore it is important to understand the reactions that can occur when SO_2 is co-injected with CO_2 (geologic co-sequestration). We are performing geochemical computer modeling and laboratory experiments to understand co-sequestration in the Mississippian Madison Limestone of the Moxa Arch in SW Wyoming. Supercritical CO_2/SO_2 is injected into an ongoing brine-rock experiment from which fluid samples are collected throughout a time series. We have finished base line experiments evaluating supercritical CO_2 reactions with a Na-Ca-Cl brine (I=.52 M) and 2 different synthetic rock types; (83% dolomite, 10% calcite, 6% anhydrite, 1% pyrite) and (86% dolomite, 13% calcite, 1% pyrite). After injection, dissolved CO_2 concentration increased from 1mM to 1.27 M and pH decreased from 7.43 to 6.35 and .78 mM to 1.22 M and pH decrease of 8.77 to 6.64. Total cation concentration increased 350% 24hr after injection then followed by a 48% decreases over 1100 hr, while the other experiment increased 1980% 24hr after injection then followed by a 40% decreases over 1080 hr. Decrease in calcium concentrations in both experiment suggest calcite precipitation, mineral trapping of CO_2. This observation coincides with secondary calcite precipitation on the Moxa Arch. The next set of experiments will incorporate minor amounts of SO_2 to see what added effects it has on the sequestration of CO_2.

Cally Driessen, M.S. Candidate
Department of Renewable Resources
Advisor: Dr. Jay Norton
Poster Presentation

METHODOLOGY AND IMMEDIATE EFFECTS OF CONTROLLED LIVESTOCK TREATMENT ON RECLAIMED NATURAL GAS WELL PADS

Cally Driessen[1], Amber Mason[2], Jay Norton[3], and Calvin Strom[4]
[1] Soil Science MS Student, Department of Renewable Resources, University of Wyoming; [2] Soil Science PhD Student, Department of Renewable Resources, University of Wyoming; [3] Assistant Professor and Extension Soil Fertility Specialist, Department of Renewable Resources, University of Wyoming; and [4]University of Wyoming Cooperative Extension Educator

Reclamation of land disturbed for energy development in Wyoming has largely been executed by extraction companies and evaluated by the governing agency. In this study, we examine an unconventional reclamation technique that aims to involve ranchers in the reclamation process: controlled livestock impact. The theory behind this technique is that by confining livestock on a seeded, reclaimed site the animals will improve the seedbed and seed to soil contact through fertilization and hoof action. Reclaimed natural gas well pads were selected from three Wyoming natural gas fields. Each well pad was given three treatment plots: traditionally reclaimed, reclaimed with the cattle impact treatment, and adjacent undisturbed. Cattle treatments were applied in fall 2009, immediately after reclamation and seeding were completed. Soil samples were taken from the undisturbed, reclaimed plots, pre-cattle treatment, and post-cattle treatment plots. Soil samples were then analyzed for soil organic matter parameters including percent soil organic fraction, soil organic carbon and nitrogen, and potentially mineralizable carbon and nitrogen. Results from the initial sampling as well as methodology will be presented. Vegetation sampling, in addition to the soil sampling, will continue throughout the 2010 growing season to determine the efficacy of controlled livestock impact as a reclamation tool.

Jessica Frint, J.D. Candidate
College of Law
Advisor: Dr. Dennis Stickley
Oral Presentation

CREATION OF UNDERGRADUATE COURSE ON ENERGY POLICY

Jessica Frint, Ben Kinney, and John Gordon

Energy policy is the means by which entities have chosen to address issues of energy development, production, distribution, and consumption. Such means can include legislation, agency regulations, and public policy determinations. This research project was conducted to create an undergraduate course that focused primarily on energy policy impacts in Wyoming. As such, nine key areas were identified, researched, and synthesized to create individual teaching/learning modules. The nine areas include Wyoming's mineral severance tax, sage grouse, social impact of energy development, carbon sequestration / coal gasification, coal bed methane produced water, in-situ uranium mining, development of a gas-fired power plant in Wyoming, transmission of wind energy, and deregulation of natural gas transmission. Each module will include introductory material, learning outcomes, summary, and potential exercises. The introductory material identifies the source of the energy policy, explains the effects of such policies, and provides additional information citations for further study. The learning outcomes are a list of objectives/concepts that each student should be able to comprehend by the completion of the module. The summary synthesizes the material in the entire module. The exercises are a series of questions designed to challenge the students understanding of the material, their ability to apply concepts learned to new scenarios or factual situations, and encourage discussions among the students. This research project created the basic foundation and structure for an undergraduate course focused on Energy Policy that can easily be changed and adapted to future instruction of the course.

Brian Gruver, Ph.D. Candidate
Department of Chemistry
Advisor: Dr. Dean Roddick
Poster Presentation

ACCEPTOR PCP CATALYSTS FOR HYDROGEN TRANSFER

Late-transition metal complexes incorporating a PCP "pincer" ligand motif have received increasing attention as catalysts for alkane dehydrogenation, with iridium systems being the most active of those systems studied thus far. Despite considerable recent interest in group 9 chemistry, nothing has been reported for alkane dehydrogenation activity of the d^6 systems. Hence, we are interested in extending PFAP (perfluoroalkylphosphine) pincer chemistry to group six metals. The acceptor ^{CF_3}PCPH ligand reacts with $[Ru(cod)Cl_2]_n$ to give the 6-coordinate anionic complex $[(^{CF3}PCP)Ru(CO)Cl_2]^-[NEt_3H]^+$. The tricarbonyl cation $[(^{CF3}PCP)Ru(CO)_3]^+[\ B(C_6F_5)_4]^-$ was prepared and isolated on a preparative scale. Though the *trans* CO arrangement is not preferred, the complex is surprisingly stable. Further reactivity suggests $[(^{CF3}PCP)Ru(CO)_3]^+[B(C_6F_5)_4]^-$ may hold promise as a decarbonylation catalyst. $[Et_4N]_2OsCl_6$ reacted with ^{CF_3}PCPH in the same manner as the corresponding ruthenium complex to give the first osmium-based ^{CF_3}PCP complex $[HNEt_3][(^{CF_3}PCP)Os(CO)Cl_2]$. Catalysts of $(^{CF_3}PCP)M(X)$ and

(^{CF_3}PCP)M(L)$^+$ types should prove advantageous over (^{CF_3}PCP)Ir catalysts. The presence of an extra X or L ligand in the active fragment provides potential for both steric and electronic tuning of the system. Overall efficiency of catalysis depends on a series of interdependent and finely balanced elementary steps, so fundamental reactivity studies will be required to resolve these issues.

Ping Guo, Ph.D. Candidate
Department of Computer Science
Advisors: Dr. Liqiang Wang and Dr. Po Chen
Poster Presentation

MODEL-BASED PARTITIONING AND AUTO-TUNING FOR SPARSE MATRIX-VECTOR MULTIPLICATION ON GPU

Ping Guo, He Huang, Oichang Chen, Liqiang Wang, Department of Computer Science
En-Jui Lee, Po Chen, Department of Geology & Geophysics

Sparse matrix-vector multiplication (SpMV) is essential for many scientific and engineering applications. The Graphics Processing Unit (GPU) is specifically designed to provide high throughput using many-core chips. Due to its massive processing capability, GPU has become an attractive coprocessor for general purpose computing. This poster presents a model-based scheme for partitioning and compressing sparse matrix in appropriate formats, and auto-tuning configuration of CUDA kernels in order to obtain optimal performance of SpMV on GPUs. Our model can predict the performance of CUDA kernels for SpMV. Based on the performance model, the auto-tuning framework can partition the original sparse matrix to sub-matrices with different storage formats and automatically adjust CUDA-specific parameters for optimal performance on specific GPUs. This work is advised by Dr. Liqiang Wang in the Department of Computer Science and Dr. Po Chen in the Department of Geology and Geophysics.

Steven Hansen, Ph.D. Candidate and Amit Padhi, Ph.D. Candidate
Department of Geology and Geophysics
Advisors: Dr. Ken Dueker and Dr. Subhashis Mallick

ADVANCES IN THE DETECTION AND MONITORING OF SUBSURFACE FORMATIONS CONTAINING SEQUESTERED CO_2 USING SEISMIC DATA

Steven Hansen and Amit Padhi

Inversion of seismic waveform data in the offset-domain suffers from the problem of aliasing since receiver spacing does not sufficiently sample the surface wavefield. To avoid this problem, data are transformed to the angle-domain and compared with synthetic data, inverting for subsurface properties. Current industry methods for offset-to-angle transform suffer from NMO stretch at longer offsets. Far-offset inversion of multi-component data is required for reliable estimates of density, which is the appropriate attribute for mapping a subsurface CO_2 plume. A ray based offset-to-angle transform method has been developed and tested for inversion of P-wave data acquired from marine surveys. This method incorporates a Genetic Algorithm waveform inversion scheme and shows promising results for velocity estimation in the water column. Similarly, it should be possible to estimate density using this technique. Another method for estimating subsurface properties is to model the amplitudes of reflected waves generated at a layer interface at different offsets. A numeric method is developed to calculate reflection coefficients for two generally anisotropic mediums. Our algorithm is checked against analytic results for isotropic and VTI mediums and results for more complicated media are presented. An important application of this research is the detection and identification of fracture sets.

He Huang, Ph.D. Candidate
Department of Computer Science
Dr. Liqiang Wang and Dr. Po Chen
Oral Presentation

A PERFORMANCE MODEL FOR SPMV KERNELS ON GPU

He Huang, Ping Guo, Oichang Chen, Liqiang Wang, Department of Computer Science
En-Jui Lee, Po Chen, Department of Geology & Geophysics

Sparse matrix-vector multiplication (SpMV) kernels on Graphics Processing Unit (GPU) are widely used in scientific computation because of its high efficiency and low costs. Estimating the execution time of SpMV kernel on GPU is the premise for kernel optimization and load-balancing. However, estimating performance is extremely difficult due to the complex hierarchy of memories in GPU. In this presentation, we will show a model-based approach to attack this problem. Our model is parameterized with configurations of GPU, arguments of kernel code, and the sizes of problems. Given a specific GPU hardware, predefined small unit matrices are tested in real executions to instantiate some parameters in the model. Finally, we estimate the execution time for any given sparse matrix by approximating its partitions to the unit matrices. The preliminary experiment shows that the execution time predicted by our model matches the real execution time of SpMV GPU kernel. This work is advised by Dr. Liqiang Wang in the Department of Computer Science and Dr. Po Chen in the Department of Geology and Geophysics.

Benjamin Kinney, J.D. Candidate
College of Law
Advisor: Dr. Dennis Stickley
Poster Presentation

LEGAL RIGHTS AFFECTING WIND ENERGY DEVELOPMENT

Benjamin A. Kinney and Brian J. Marvel

Our research was focused on the various property and other legal rights that affect the development of wind energy in Wyoming. A substantial amount of this information was presented to the Wyoming State Legislature's Task Force on Wind Energy that met through the summer and fall of 2009. The information presented in this poster traces the development of a legally defined "wind right," along with an analysis of different conflicts that wind energy development may pose to the state. Specifically, we addressed the issue of "severability" of wind rights, which is the ability of the owner of the right to "sever" and sell that right. We discuss both cases in which the issue has been addressed by courts, as well as different state statutes. We also studied several other issues including land use conflicts, transmission problems, and taxation. Finally, we would include a brief discussion of recent actions by the Wyoming State Legislature regarding wind energy development and the potential impact of new laws on wind energy in Wyoming.

Joo Seob Lee, Ph.D. Candidate
Department of Chemical and Petroleum Engineering
Advisor: Dr. Patrick A. Johnson
Oral Presentation

CAPTURING CARBON DIOXIDE (CO_2) WITH ENZYMES

Joo Seob Lee and Patrick A. Johnson

Global climate change is a large threat due to excessive human emissions of green house gases, such as carbon dioxide. Thus, with the scientific and public acceptance of climate change due to anthropogenic sources, CO_2 capture has attracted significant interest. In this study, novel materials have been fabricated with the enzyme, carbonic anhydrase (CA), for the capture of CO_2. Specifically, carbonic anhydrase has the function to catalyze the conversion of CO_2 to bicarbonate ions. In the process, the bicarbonate anion could be coupled with a positively charged ion to form bicarbonate salts or reacted by other enzymes to form hydrocarbon products. Carbonic anhydrase was immobilized on magnetic nanoparticles (Fe_3O_4) as well as in PVA coated magnetic nanoparticles (PVA-MNPs). Consequently, enzymes immobilized on magnetic materials (CA embedded on PVA-MNPs) were fabricated. The novel materials were characterized by Fourier Transform Infrared Spectrometry (FT-IR), Differential Scanning Calorimetry (DSC), zeta-potential measurements, Dynamic Light Scattering (DLS), Transmission Electron Microscopy (TEM), UV-Vis spectrometry and Stability Test (ST) for storage in aqueous solution. Therefore, we expect that this study can give insights in development of enzyme immobilized nanoparticles to facilitate the conversion of CO_2 to bicarbonate.

Liyou Lu, Ph.D. Candidate
Department of Physics and Astronomy
Advisor: Dr. Wenyong Wang
Poster Presentation

SYNTHESIS OF ZNO AND ITS TERNARY CONMPOUND NANOWIRES USING THE PULSED LASER DEPOSITION TECHNIQUE

Liyou Lu and Wenyong Wang

In the past decade there has been significant research interest on nanostructures especially on nanowires due to their special structural and transport properties. Metal oxide nanowires including ZnO and its ternary compounds are promising candidates for electronic and opto-electronic device applications, such as field-effect transistors or photovoltaic devices. In this research we investigate the growth of ZnO and Zn_2SnO_4 nanowire arrays using the pulsed laser deposition (PLD) technique. PLD is a powerful tool for the growth of high quality crystalline thin films, and it recently has been utilized to synthesize semiconductor nanowires. However, the mechanisms of nanowire growth of different materials using PLD are not fully understood. In order to achieve a better understanding of the PLD growth process, we investigate the effect of different growth parameters, such as chamber pressure, substrate temperature, catalyst material, etc., on the structural and morphological properties of the nanowires. X-ray diffraction (XRD) and Scanning Electron Microscopy (SEM) are used for the examination of these properties. The research on the application of metal oxide nanowires in power conversion devices such as dye-sensitized solar cells will proceed after the successful synthesis of these materials.

Yitong Luo, M.S. Candidate
Department of Civil and Architectural Engineering
Advisor: Dr. David Bagley
Poster Presentation

BIO-HYDROGEN PRODUCTION FROM CASEIN USING DARK FERMENTATION PROCESS

Dairy wastewater is composed of easily degradable carbohydrates, mainly lactose, as well as proteins and lipids. Casein is the major protein in milk (almost 80% of the total proteins) and in dairy effluents. Anaerobic fermentative processes have been examined to produce hydrogen with glucose providing hydrogen yields around 2.0-2.4mol/mol glucose. During anaerobic fermentation of dairy wastewater to produce bio-hydrogen, lactose should readily ferment. The fermentation of casein to produce bio-hydrogen has not been examined, however. Therefore, the objective of this research is to determine the hydrogen production potential from casein.

This research is conducted in both batch and continuous reactor experiments. In the batch experiment, 160-mL serum bottles were inoculated with anaerobic digester sludge from the Cheyenne Dry Creek municipal wastewater treatment plant. Glucose and casein were added to achieve 500mg/L COD. Autoclaved and non-autoclaved bottles were incubated with a pH of 5.5 at 30ºC. Headspace analysis with gas chromatography provided gas composition and production measurements. In the bottles receiving casein, the maximum hydrogen production in autoclaved bottles was 150μmol/bottle compared to 15μmol/bottle in non-autoclaved bottles. In the bottles receiving glucose, hydrogen production in the non-autoclaved bottles was 210μmol/bottle.

The continuous reactor experiments are currently underway using a customized 4-L aspirator glass bottle with pH control to 5.5 and incubated at 30ºC. The first step is to determine an appropriate hydraulic retention time (HRT) to sustain hydrogen production from casein. Preliminary results suggest that an 8 h HRT may be too short. In addition to hydrogen production, protein and chemical oxygen demand will be measured as well as ammonia and volatile fatty acid production. This reactor could serve as the first step in a two-stage process, with the second stage consisting of a photofermentation process that converts produced volatile fatty acids into hydrogen and carbon dioxide. Continuous reactor data are expected to be available by May.

Amber Mason, Ph.D. Candidate
Department of Renewable Resources
Advisor: Dr. Jay Norton
Poster Presentation

NITROGEN DYNAMICS OF NATURAL GAS TOPSOIL STOCKPILES

<u>Amber Mason</u>, Cally Driessen and Jay Norton

In recent years, natural gas extraction activities have disturbed thousands of acres of arid and semiarid regions in Wyoming’s sagebrush steppe ecosystem. Thin, nutrient poor topsoils, combined with subsoils potentially high in salts, limit the resilience of these arid and semiarid soil systems. Stripping and stockpiling topsoil stimulates decomposition and loss of soil organic matter (SOM) by breaking apart soil structure and eliminating inputs of plant residues, which can result in reduced SOM content. Preliminary data suggests that the soil organic matter that is needed for plant growth becomes mineralized or released when the soil is disturbed. The data shows a small increase in mineral N concentrations after stripping and stockpiling compared to undisturbed soils. The spike in mineral N originates from organic compounds that, in undisturbed conditions, hold and slowly release N and other nutrients. It represents a significant potential loss of this important “time-release” nutrient pool. The purpose of this study is to gain an understanding of how natural gas development and reclamation activities impact soil properties.

Dawei Mu, Ph.D. Candidate
Department of Geology and Geophysics
Advisor: Dr. Po Chen
Oral Presentation

AN ARBITRARY HIGH ORDER DISCONTINUOUS GALERKIN METHOD FOR ELASTIC WAVE ON UNSTRUCTURED MESHES

This article presents a new numerical scheme to solve the elastic wave equation in heterogeneous media with arbitrary high order accuracy in space and time on unstructured tetrahedral meshes. This method combines a discontinuous Galerkin (DG) method with the ADER time integration approach using Arbitrary high-order DERivatives. The DG-ADER scheme helps reduce the numerical approximation errors while retain high order accuracy both in space and time, unstructured tetrahedral mesh makes it can handle complicated geometry. Furthermore, the projection of the tetrahedral elements in physical space on to a canonical reference tetrahedron allows for an efficient implementation, as many integrals can be analytically pre-computed. However, with the increasing complexity of the unstructured tetrahedron mesh and the accuracy require, the huge computation amount was not affordable by traditional CPU system, therefore, using the GPU technology to implement the DG-ADER scheme on GPU system to complete the computational task could be an efficient and effective solution of this problem, since the GPU enjoys many merits which specially suit for scientific parallel computing. Therefore, applying DG-ADER scheme with this advanced architecture is the other goal for this project.

Saeed Ovaysi, Ph.D. Candidate
Department of Chemical and Petroleum Engineering
Advisor: Dr. Mohammad Piri
Oral Presentation

DIRECT PORE-LEVEL MODELING OF INCOMPRESSIBLE FLUID FLOW AND DISPERSION IN POROUS MEDIA: AN ADAPTIVE APPORACH

A three-dimensional fully dynamic parallel particle-based model for direct pore-level modeling of incompressible viscous fluid flow in disordered porous media is presented. The model was developed from scratch and is capable of simulating flow directly in three-dimensional high-resolution micro-CT images of rock samples. The model is based on Moving Particle Semi-implicit (MPS) method. This technique is significantly modified in order to improve its stability for flow in porous media problems. The model reads the images as input where the positions of the solid walls are given. The entire medium, i.e., solid and fluid, is then discretized using particles. The Navier-Stokes and continuity equations are then solved to evolve the properties, e.g., coordinates, velocity, pressure, etc., of each particle. The model handles highly irregular fluid-solid boundaries effectively. It includes a sophisticated algorithm to automatically split and merge particles to maintain hydraulic connectivity of extremely narrow conduits. To handle the computational load, a fully parallel version of the model is developed that runs on distributed memory computer clusters and exhibits excellent scalability. The model is used to simulate transient- and steady-state flow directly in REV size images of two different sandstones with 3.398 and 3.85 µm resolutions. We analyze the quality and consistency of the predicted flow behavior and calculate absolute permeability using the steady-state flow rates. We show that the model conserves mass very well and is stable computationally. The model is then used to study solute transport directly in high- resolution micro-CT images of Berea sandstone. The predicted dispersion coefficients are compared successfully against the experimental data available in the literature. To the best of our knowledge, this is the first direct three-dimensional particle-based pore-level model of flow of an incompressible fluid in porous media that directly solves the Navier-Stokes and continuity equations for each fluid particle in parallel.

V. K. Chaitanya Pakala, Ph.D. Candidate
Department of Mechanical Engineering
Advisor: Dr. O.A. "Gus" Plumb
Oral Presentation

HEAT TRANSFER AT AN EVAPORATING FRONT IN POROUS MEDIA – AN EXPERIMENTAL STUDY

Evaporating fronts propagate through porous media during drying processes, underground coal gasification (UCG), geothermal energy production from hot dry rock, and around nuclear waste repositories. In this presentation the advantages and disadvantages of UCG will be explored. The importance of the heat and mass transfer at the interface between hot gases and water saturated porous media will be discussed. The presentation will focus on the one-dimensional heat transfer at the interface between vapor saturated porous matrix and water saturated porous region, experimental observations will be reported for an evaporating front that develops in a vertical cylinder heated from below. The cylinder is filled with water-saturated porous materials. A porous plate is attached in the cylinder at the bottom and is equipped for vapor flow as and when it develops, and this is controlled manually. The author will discuss preliminary experimental results and compare with existing experimental data.

Hee Joon Park, Ph.D. Candidate
Department of Chemical and Petroleum Engineering
Advisor: Dr. Patrick A. Johnson
Oral Presentation

SYNTHESIS AND CHARACTERIZATION OF B-GLUCOSIDASE (EC 3.2.1.21) BIOCONJUGATE ON MAGNETIC NANOPARTICLE FOR BIOCATALYST APPLICATION

Hee Joon Park[1], Ashley Driscoll[1], Matt Kipper[2], Patrick Johnson[1]*
Department of Chemical and Petroleum Engineering at University of Wyoming[1]
Department of Chemical and Biological Engineering at Colorado State University[2]

Four different types of bioconjugates were developed using magnetic nanoparticles (MNPs) as a core solid supports and β-glucosidase (βG) as the immobilized enzyme. MNPs were prepared by oxidation of $Fe(OH)_2$. βG was covalently bound on the surface of MNPs by two different methods. The first method used glutaraldehyde as a cross-linking agent between amine groups on MNP and enzymes. MNP surfaces were modified with 3-(aminopropyl)triethoxysilane (APTES) to express amine groups on the surface. The second method adds poly(ethylene glycol) (PEG) as a longer spacer between MNPs and βG. The surface of MNPs were functionalized with (3-glycidyloxypropyl)trimethoxysilane (GOPES) which has an epoxide ring at the end, then three different molecular weight PEGs (200, 400, and 1000) were anchored to the epoxide ring. The saturated magnetization (Ms) of fresh made MNPs was 62.3 emu g^{-1} and was reduced to 60.4 emu g^{-1} after the immobilization process. The amount of protein immobilized on the MNPs was estimated by the BCA assay and was approximately 12.6 – 15.4%. The bioconjugates were thermally stable at 65 ^oC and tested for five consecutive recycling processes. In terms of product conversion, the substrate conversion quantity of bioconjugates was comparable to native βG after the fifth recycling round.

Sarah L. Ramsey-Walters
Ph.D. Candidate in Education and M.S. Candidate in Natural Sciences
College of Education
Advisor: Dr. Robert Mayes
Oral Presentation

SUPPORTING K-12 ENERGY EDUCATION

K-12 energy education is currently under review throughout Wyoming to support local programs. The statewide review includes a teacher survey to better understand the status of energy and environment education and the barriers to effective curricular implementation. In addition to the energy survey, a literature review of energy education best practices and existing national programs will provide a foundation for professional development programs and curricular resources to meet the needs of Wyoming teachers. Currently, a curricular resource database is available to teachers and future work will be driven by identified needs to support energy and environment education in Wyoming.

Gevorg Sargsyan, Ph.D. Candidate
Department of Chemistry
Advisor: Dr. Milan Balaz
Oral Presentation

DNA-PORPHYRIN ASSEMBLIES FOR LIGHT HARVESTING AND ENERGY TRANSFER

Gevorg Sargsyan and Milan Balaz

Self-assembled multichromophore systems have recently become one of the most important and attempted approaches in the field of artificial light harvesting systems. The aim of this project is to design and synthesize covalent supramolecular DNA-metalloporphyrin assemblies for light-harvesting and energy transfer. Porphyrins, due o their high stability and efficient light absorbance in the visible part of the spectrum, are extremely suitable and important building blocks for construction of covalent and supramolecular light-harvesting systems. Porphyrins will be assembled on DNA scaffold thus combining the advantages of covalent (precise) and supramolecular (flexibility) approaches for preparing energy transfer systems. The structural flexibility of our assemblies combined with the possibility to easily modify the electronic properties of the chromophores will provide us with a unique opportunity to obtain a detailed knowledge of photophysical processes involved in light absorption and energy transfer. By varying the sequence and the structure of DNA, the energy transfer and migration between metallo- and free-base porphyrins will be explored as a function of distance and arrangement of the chromophores.

William C. Schaffers, Ph.D. Candidate
Department of Chemical and Petroleum Engineering
Advisor: Dr. David Bell
Oral Presentation

COAL FIRED IGCC POWER PLANTS IN WYOMING

William C. Schaffers, Dr. David Bell (University of Wyoming) and Dr. Richard Boardman (Idaho National Laboratory)

Coal fired Integrated Gasification Combined Cycle (IGCC) power plants may become an important power source if carbon dioxide emission regulations are implemented. These plants allow for the production of a more concentrated CO2 stream already under some pressure. Further compression and sequestration of the CO2 is thus more economical than with conventional coal fired plants. In addition, it is possible to combine IGCC plants with other types of chemical or fuel plants to utilize the synthesis gas produced in the gasifier. This study compares IGCC power plants utilizing slurry and dry fed gasifiers at various levels of CO2 capture. The purpose is to determine how the configurations respond to the use of Powder River Basin coal. An additional comparison was made utilizing air cooling rather than the conventional water cooling and with a high rate of water recycle. Such a configuration is likely to become more attractive due to increasing demands on Wyoming's limited water supply.

Michael Stoellinger, Ph.D. Candidate
Department of Mathematics
Advisor: Dr. Stefan Heinz
Oral Presentation

PROGRESS POTENTIAL FOR CLEAN COAL TECHNOLOGY

Numerical simulations of coal combustion and gasification processes offer great potential for analyzing, designing and optimizing the performance these processes. This is due to the extremely detailed, multi-dimensional information provided by comprehensive numerical simulations which cannot be obtained from experiments. A comprehensive model for coal gasification contains a large number of sub-models which embody the mathematical and numerical characterization of the fundamental principles that characterize the complex physical and chemical phenomena of interest. These sub-models and their interconnection will be presented. The comprehensive model for coal gasification will be validated by comparing simulation results for a pilot scale coal furnace to measurements.

Thomas C. Sturtevant, M.S. Candidate
Department of Atmospheric Science
Advisors: Dr. Robert Field and Dr. Derek C. Montague
Oral Presentation

UPPER GREEN RIVER VALLEY OZONE INVESTIGATION

Ozone is a secondary air pollutant regulated through the National Ambient Air Quality Standards of the Clean Air Act, as exposure can lead to health risks. Over the past five years, elevated ground-level ozone (O_3) concentrations have been observed during winter in the Upper Green River Valley (UGRV) of western Wyoming. Substantial oil and gas development has occurred in the region during this period. These O_3 episodes appear to be associated with distinct meteorological conditions such as synoptic high pressure, clear skies, snow cover, low wind speeds, and temperature inversions. Formation of O_3 largely

occurs through a photoinitiated reaction sequence involving the oxides of nitrogen and non-methane hydrocarbons (NMHC), which are emitted in the region in parallel to methane emissions. During the winter of 2008/09, monitoring of ozone was performed at five UGRV observation sites using commercial ozone and ozone-precursor monitoring instrumentation installed in a mobile laboratory along with a standard suite of meteorological instrumentation. Wind and pollution roses constructed from the analyzed data depict site-specific regimes at each location, with evidence of localized transport of emissions from nearby sources. Peak concentrations of ozone usually occur in the afternoon, whereas those for methane/NMHC tend to occur in the early morning.

Xiuyu Wang, Ph.D. Candidate
Department of Chemical and Petroleum Engineering
Advisor: Dr. Vladimir Alvarado
Oral Presentation

INTERFACIAL PROPERTY ANALYSIS OF WATER-IN-CRUDE OIL EMULSION STABILITY AND ITS IMPLICATIONS IN ENHANCED OIL RECOVERY

Xiuyu Wang and Vladimir Alvarado

The stability of water-in-oil emulsions is controlled by either the oil film rheology between approaching drops or/and by the strength of drop interfaces. Film drainage is mainly a function of the continuous phase viscosity. In this study, one crude oil is used to formulate water-in-oil emulsions. Temperature is regulated to control the viscosity of the continuous phase and hence determine its effect on emulsion stability through film drainage, in contrast with interfacial strength control. Cation type in the brine, which could affect emulsion stability, is examined by comparing the stability of emulsions made with either purely monovalent or divalent brines with the same overall ionic strength.

Water-in-crude oil emulsions can possibly form during oil production, especially when EOR methods are applied, such as ASP and LoSal™ water flooding. The pros and cons of emulsion formation have thus motivated significant research work in the oil industry.

It is observed that divalent cations in the brine contribute to form stronger emulsions than those produced with purely monovalent brines. The critical field value, used as proxy of emulsion stability, reaches a plateau at sufficiently high temperature (50 ^{o}C), which we interpret to be the intrinsic drop-coating film resistance to rupture. From the comparison with previous results with a less asphaltic oil, we speculate that the drop coating film is composed of a fraction of asphaltenes. Designed oil wash tests, being a new and straightforward experimental method in studying mechanism of crude oil emulsion stability, has shown a trend of continuously depletion of surface active components from the oil corresponding to decreased emulsion stability determined from electrorheological test.

The ultimate objective of this study is to better understand the formation of water-in-crude oil emulsions by analyzing important parameters affecting emulsion stability, such as temperature, oil composition and rheology, aqueous phase salinity and cation type. From this work, it is hoped the conditions that promote recovery based on emulsions for existing EOR methods can be engineered.

Qing Zhang, M.S. Candidate
Department of Civil and Architectural Engineering
Advisor: Dr. Ahmed C. Megri
Oral Presentation

RETROFIT OF HVAC COMMERCIAL BUILDING USING VAV SYSTEM INTEGRATED WITH THERMAL STORAGE SYSTEM

Zhang Qing, Jay Puckett, Anthony Denzer, and Ahmed C. Megri

With the cost of electricity constantly rising, energy conservation opportunities become ever more attractive. Green building grabs all the headlines, but retrofitting existing buildings is where the real savings are for most buildings. In this work, an existing commercial building has been retrofitted. Multiples measures have been considered to improve the energy efficiency, as well as the thermal comfort of the building. This work describes a proposed energy-efficient retrofit of a heating, ventilating, and air-conditioning system for a commercial building from constant volume to variable air volume using TRNSYS program. A parametric study has been performed to select the most appropriate and efficient configuration. Many systems have been investigated including geothermal heat pump (GHP) system, thermal energy storage systems for cooling and heating, as well as solar energy. Measures to improve the energy efficiency, such as the retrofit form constant volume to variable air volume system, the use of variable speed drives for variable air volume fans have been implemented on an existing commercial building. The integration of these measures with other energy storage systems has been investigated.