# **Oil & Natural Gas Technology**

DOE Award No.: DE-FE0001243

# Clean and Secure Energy from Domestic Oil Shale and Oil Sands Resources

# Quarterly Progress Report (January – March 2012)

Submitted by: University of Utah Institute for Clean and Secure Energy 155 South 1452 East, Room 380 Salt Lake City, Utah 84112

Prepared for: United States Department of Energy National Energy Technology Laboratory

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**Office of Fossil Energy** 

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Submitted by: Institute for Clean and Secure Energy 155 S. 1452 E. Room 380 Salt Lake City, UT 84112

Principal Investigator: Philip J. Smith Project Period: October 1, 2010 to September 30, 2013

> Prepared for: U.S. Department of Energy National Energy Technology Laboratory

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#### **EXECUTIVE SUMMARY**

The Clean and Secure Energy from Domestic Oil Shale and Oil Sands Resources program is part of the research agenda of the Institute for Clean and Secure Energy (ICSE) at the University of Utah. In outreach efforts, ICSE participated in a session on oil sands at the Utah Governor's Annual Energy Development Summit on February 15, 2012. In addition, the External Advisory Board (EAB) recommendations were finalized and circulated to EAB members as well as ICSE faculty, staff and students.

Researchers in Task 3.0 are developing a modified assessment tool for evaluating regional economic and environmental effects of unconventional fuel development. Work this quarter was temporarily suspended pending the completion of the Market Assessment (Subtask 6.3) by key personnel. The Subtask 3.1 team continued to refined the transportation-related emission factors for the air quality module in the model. The Subtask 3.2 team developed a coupled approach to simulating both the 2m x 2m x 6m International Flame Research Foundation (IFRF) furnace and the TEA-C burner that it is fired with. This approach involves fully resolving the burner geometry and the fluid flow through that geometry in Star-CCM+ and then using the simulation outputs at the exit plan of the burner as the inputs for the ARCHES simulation of the furnace.

A wide range of analyses on three different sections of the Skyline 16 core (GR-1, GR-2, and GR-3) were conducted as part of Subtasks 4.3, 4.5, 4.6, 4.7, 4.8, and 4.9 during this guarter. The Subtask 4.3 researchers conducted thermogravimetric analysis (TGA) experiments at three different heating rates (5°C/min, 10°C/min and 20°C/min) with kerogens extracted from homogenous powdered samples of GR-1, GR-2 and GR-3 oil shales. They also continued collection of tar and char samples from the same demineralized kerogen samples from Green River Basin using the kerogen retort. The Subtask 4.5 team compared the texture change of kerogen-rich GR-1 core samples before and after pyrolysis at different reaction temperatures (450°C and 500°C) and a heating rate of 100°C/min by comparing the relative position of mineral grains. Additionally, directional permeability of GR-1 cores was calculated based on the pore network structure from X-ray computed tomography analysis coupled with LB simulation. Subtask 4.6 researchers modeled the interaction of kerogen with mineral matrices, using fragments of published crystal structures of illite, dolomite and calcite. The calculations were completed at the molecular mechanic level of theory using the UFF potential available in Gaussian 09. Subtask 4.7 researchers focused on design modifications and added capabilities for the apparatus they will be using for in situ testing of GR-1, GR-2 and GR-3 core samples. They also obtained permeability and porosity measurements of the oil shale samples that will be used in the in-situ testing simulations. These measurements were performed gratis by TerraTek. The Subtask 4.8 team performed a Quantitative Evaluation of Mineral by SCANning electron microscopy (QEMscan) analysis and determined that the mineralogic textures are dominated by dolomite, illite, and calcite. The Subtask 4.9 research team completed data collection on the kerogen and bitumen extracted from GR-1, GR-2, and GR-3, including small angle x-ray scattering and atomic pairwise distribution functions and bitumen solution NMR.

The other Task 4.0 projects are focused on simulation of various in situ processes. The Subtask 4.1 team added a reaction chemistry model and improved oil shale properties to the Star-CCM+ CFD-based simulation tool they are developing to study the thermal heating of oil shale inside the Red Leaf ECOSHALE capsule. They can now study product yield as a function of temperature and of shale properties. The Subtask 4.2 team studied a method for reducing computational cost and increasing accuracy of simulation results. This method uses random data sampling combined with the Central Limit Theorem to propagate error through dynamic calculations.

Subtask 5.0 researchers have completed and submitted a topical report on cross-jurisdictional resource management. Only Subtask 5.3 remains to be completed. In Task 6.0, six sections of the Market Assessment are ready for publication and a seventh section is in the page layout phase of preparation. Three sections remain to be finalized and to be prepared for publication.

American Shale Oil (AMSO) and Task 7.0 researchers are working together to advance the AMSO technology for in situ production of shale oil. A biweekly progress report is circulated to team members in addition to regularly scheduled meetings held on the University of Utah campus. The Subtask 7.2 team coupled a K-value based thermal reservoir model and a geomechanical model in the framework of the Advanced Reactive Transport Simulator to perform the reservoir simulation of coupled geomechanics for a thermal recovery process. Subtask 7.3 researchers studied the effects of the crack size on the thermal history and distribution inside a representative oil shale bed geometry. They have created a suite of simulations of varying crack sizes, and have quantified the effects of crack size on the thermal distribution for one of the scenarios being tested. Team members are working with AMSO scientists to replicate their experiment as closely as possible.

#### PROGRESS, RESULTS, AND DISCUSSION

#### Task 1.0 - Project Management and Planning

During this quarter, there were no schedule/cost variances or other situations requiring updating/amending of the PMP.

#### Task 2.0 -Technology Transfer and Outreach

Task 2.0 focuses on outreach and education efforts and the implementation of External Advisory Board (EAB) recommendations. During this quarter, the 2011 EAB recommendations were finalized and circulated to EAB members as well as ICSE faculty, staff and students. A copy of the final recommendations is attached as Appendix A. Planning also began in this quarter for the 2012 University of Utah Unconventional Fuels Conference. This conference has evolved over the years from a conference focusing strictly on oil sands to a conference that considers the range of unconventional fuels of interest to stakeholders in the state of Utah and in the western U.S. This year's conference is co-hosted by the State of Utah's Office of Energy Development.

#### Task 3.0 - Clean Oil Shale and Oil Sands Utilization with CO<sub>2</sub> Management

#### Subtask 3.1 (Phase I) – Macroscale CO<sub>2</sub> Analysis (PI: Kerry Kelly, David Pershing)

Completion of the Phase 1 milestone is still delayed while results for the four oil shale and oil sands development scenarios are completed. Subtask 3.1 researchers anticipate receiving updated results by the end of February and expect to complete this task by March 2012.

## Subtask 3.1 (Phase II) – Lifecycle Greenhouse Gas Analysis of Conventional Oil and Gas Development in the Uinta Basin (PI: Kerry Kelly, David Pershing)

During this quarter, the project team refined the transportation-related emission factors based on comments from members of related tasks. Team members continue to monitor several potentially useful sources of validation data for greenhouse gases that will be released in the coming months, including the Bureau of Land Management's air emissions inventory and the Uintah Basin air emissions inventory update being developed by Utah State University. Finally, revisions were made to this task's contribution to the Assessment because of the evolving regulations on low-carbon fuel standards.

This project's milestone, the submission of a joint publication with Subtask 6.2, is delayed until they finish the Assessment.

#### Subtask 3.2 - Flameless Oxy-gas Process Heaters for Efficient CO2 Capture (PI: Jennifer Spinti)

The Subtask 3.2 team has been taken a coupled approach for performing the simulations of the IFRF's oxy-gas experiments (Coraggio and Laiola, 2009). Preliminary simulations made it clear that getting the detailed geometry of the burner correctly modeled was essential in capturing the species concentrations and temperature fields in the near burner region of the furnace. The ARCHES LES code can resolve the dynamics of the flame in the large domain of the furnace (2m x 2m x 6m) but cannot resolve the swirl vanes, gas nozzles, etc. in the burner due to the prohibitive computational cost of resolving such small scales in such a large computational domain. The commercial CFD software Star-CCM+ can resolve the burner geometry so that flow velocities at the exit plane of the burner can be computed but cannot properly account for radiative heat loss in the near burner region. The project team decided to take a coupled approach by creating the complex TEA-C burner geometry in Star-CCM+. Using this geometry, a Star-CCM+ simulation of flow through the burner produced velocities of fuel and oxidant flows at the exit plan of the burner. This information was then used as an input to a non-reacting ARCHES simulation using the IFRF furnace geometry. Figure 1 shows a volume-rendered image of the resulting vorticity field in the furnace. This methodology appears to produce stable ARCHES solutions, so the project team will be able to move forward with completing a similar test for a reacting flow case and then running the matrix of simulations needed for the V/UQ analysis.



**Figure 1**: Vorticity field from ARCHES simulation of the oxy-gas fired IFRF furnace with burner inlet conditions from STAR-CCM+ simulation of TEA-C burner.

The graduate student working on a flamelets reaction model with scale separation of the reaction chemistry (slow reaction solved on the mesh, fast reactions solved at the subgrid scale) had his thesis defense during this quarter and has accepted a job. He completed some parts of the project, but a new student, Alex Abboud, has been recruited to finish up the incomplete portions of the project.

#### Subtask 3.3 - Development of Oil and Gas Production Modules for CLEAR<sub>uff</sub> (PI: Terry Ring)

There was no work performed on this project during the quarter due to time commitments with Subtask 6.3 on the part of team members.

#### Subtask 3.4 - V/UQ Analysis of Basin Scale CLEARuff Assessment Tool (PI: Jennifer Spinti)

The PI of this subtask, Jennifer Spinti, attended the Black Wax Workshop help in Vernal, Utah on April 12, 2012. Presentations were given by various Salt Lake City refiners, Uinta Basin producers, and government regulators. Based on the material that was presented with respect to the labor costs for producing black wax crudes versus conventional crudes, the project team will need to include an additional "black wax" well type in the models that is being developed.

There was no work performed on this project during the quarter due to time commitments with Subtask 6.3 on the part of team members.

#### Task 4.0 - Liquid Fuel Production by In-situ Thermal Processing of Oil Shale/Sands

Subtask 4.1 (Phase I) - Development of CFD-based Simulation Tools for In-situ Thermal Processing of Oil Shale/Sands (PI: Philip Smith)

The Subtask 4.1 team submitted a topical report that details the heat transfer process inside the representative computational geometry. The report was approved by Robert Vagnetti during this quarter.

Subtask 4.1 (Phase II) - Development of CFD-based Simulation Tools for In-situ Thermal Processing of Oil Shale/Sands (PI: Philip Smith)

The Subtask 4.1 team is using the commercial software Star-CCM+ to develop highperformance computing (HPC) CFD-based simulation tools to study the thermal heating of oil shale inside the ECOSHALE capsule developed by their industrial partner Red Leaf Resources. During this quarter, team members have refined shale properties and expanded their modeling to include reaction chemistry in order to study product yield as a function of temperature, thus completing a milestone that was due in February 2012.

In previous quarterly reports, Subtask 4.1 researchers have described in detail the geometry creation process used to approximate the rubblized pieces of oil shale inside the Star-CCM+ computational domain. In this past quarter, they have identified several scientific papers that describe fundamentals of oil shale kinetics, including first order reaction models – Campbell et al. (1978), Sweeney et al. (1987), Granoff and Nuttall (1978), and Allred (1966). Researchers have focused on the work of Campbell et al. (1978) as it provides experimental results for a simplified case of heating a solid block of oil shale.

Using the experimental setup described in Campbell et al. (1978), the Subtask 4.1 team has created a computational domain representing 90 grams of oil shale. The oil shale kinetics and properties as described in the paper have also been implemented, and the bottom boundary condition is assumed to be the heating source. Simulation results (e.g. the temperature field) obtained by the heating of the small block of shale for 1,200 seconds are shown in Figure 2. With the implementation of oil shale kinetics, the production of oil as a function of time from this small block of shale is computed. The results in Figure 3 show that 7 grams of oil are produced; Campbell et al. (1978) report 6 grams of oil produced. This discrepancy could arise from the inaccurate representation of boundary conditions in the STAR-CCM+ simulations in comparison to the experiment. However, team members were unable to locate all of the information needed for an exact comparison.



Figure 2: Computation representation of the experiment conducted by Campbell et al. (1978).



Figure 3: Oil production from the simulation of a heated 90-gram oil shale sample.

In the next quarter, team members plan to refine simulations of the experiment conducted by Campbell et al. (1978) and to apply the tools that have been developed to the ECOSHALE process used by Red Leaf Resources.

#### Subtask 4.2 - Reservoir Simulation of Reactive Transport Processes (PI: Milind Deo)

In the this quarter, the Subtask 4.2 team looked at some fundamental ways by which to identify important parameters and generate response surfaces. The milestone to incorporate advanced kinetic and composition models for oil shale pyrolysis into commercial and new compositional reservoir simulators has been developed in concept but will not be completed until next quarter.

In situ oil shale process modeling requires complex models that are capable of representing several physical phenomena at widely varying time and length scales. Data for input into models and for model validation purposes are expensive and sparse. High levels of variation in input data within a physical system add additional challenges because the required resolution of the data incorporated into a model is uncertain. A common approach for improving modeling accuracy for complex systems such as in situ oil shale production processes is to add all physical processes judged to be important, compare solutions to experimental or historical data, and refine the tool by adjusting physical models or solution methods. Throughout this iterative process, the awareness of the balance between computational cost and required solution accuracy is an important challenge. In other words, some development of modeling tools may add computational cost with marginal (or unknown) solution improvement. Also, when additional parameters and complexity are introduced into a modeling tool, these parameters can be massaged to fit historical, analytical, or experimental data without true understanding of what is controlling the experimental observations or the data provided by the modeling tool.

An alternative development approach to address these issues has been a topic of this research. A method using random data sampling combined with the Central Limit Theorem for making calculations and propagating error through dynamic calculations has been demonstrated with a prototype one dimensional heat conduction problem. The heat conduction problem is shown in Equation (1).

$$\frac{\partial T}{\partial t} = \alpha \frac{\partial^2 T}{\partial x^2} \tag{1}$$

Using a finite difference method with a forward Euler approach and Dirichlet boundary conditions, the solution shown in Figure 4 is calculated.



Figure 4: Solution to one-dimensional heat conduction problem.

If all solution points are assigned an initial guess of 25 temperature units and then randomly sampled using Equation (2), the solution shown in Figure 5 is calculated. Note that Equation (2)

implies that the temperature at a point in time is dependent on a temperature gradient, elapsed time, and distance.





Figure 5: Solution to the heat equation using the sampling equation.

While this solution appears quite different from the finite difference solution, some of the characteristics are the same. They both approach the equilibrium condition advancing forward in time, and the center point does not change. If the initial guesses of 25 temperature units are disregarded and the solutions are calculated at early times first, the solution shown in Figure 6 is calculated.



Figure 6: Solution to the heat equation using the sampling equation with solutions calculated at early times first.

Again, the solution is different, but some characteristics of the solution are the same. This third solution initially shows a faster rate for approaching the steady state solution than the second

solution, when only the sampling strategy was changed. A histogram of the sample means can be plotted at any point in time to estimate the calculated uncertainty as shown in Figure 7.



#### Figure 7: Histogram of sample means.

The quality of the solution using this method depends on the number of samples calculated, the sampling model, and the sampling strategy. The benefits of this approach are that uncertainty can be propagated through calculations. Also, the more calculations that are made, the better the solution will be, so ideally the balance between computational cost and solution improvement will be more straightforward than with other modeling approaches.

#### Subtask 4.3 - Multiscale Thermal Processes (PI: Milind Deo, Eric Eddings)

The milestone to complete core sample pyrolysis at various pressures and to analyze product bulk properties and composition was not completed due to equipment malfunctions with the thermogravimetric analyzer (TGA). Some of the equipment has now been fixed and the TGA is able to run at atmospheric pressure, but further work is needed before pressurized runs will be possible.

During this quarter, the Subtask 4.3 team continued collection of tar and char samples from Skyline 16 demineralized kerogen samples using the kerogen retort, dissolved tars collected from pyrolyzed demineralized kerogen samples, conducted TGA experiments on demineralized kerogen samples, and trained a new assistant for continuation of research in the next quarter.

Char and tar samples were collected from the demineralized Skyline 16 kerogen sample GR2.9. Samples were heated at a standard heating rate of 10 K/min to temperatures between 300°C and 575°C in the kerogen retort. Tars from each experiment were condensed on glass wool and then cooled using a dry ice/isopropanol mixture. Figure 8 shows a schematic of the reactor used to perform experiments.



Figure 8: Schematic of the kerogen retort.

Masses of each individual section of the reactor were recorded both before and after each experiment to determine yields of char, tar, and light gases. Results are plotted in Figure 9 with Figure 10 (GR1.9 results) included for comparison. Due to inaccuracy with the scale used in the beginning of this quarter, team members did not yet achieve a full plot of yield versus temperature for the GR2.9 kerogen. The limited amount of remaining sample will be used to fill in the missing data points in the upcoming quarter if time permits.



Figure 9: Partial results from pyrolysis of GR2.9.



Figure 10: Complete results from pyrolysis of GR1.9.

A complete analysis of demineralized sample GR3.9 has been started. The ash content for this sample was determined to be 4.2%. Due to the available quantity of GR3.9 sample, the project team will be able to perform duplicate experiments at the higher temperatures in order to get enough char to analyze by NMR.

SEM/EDAX X-Ray analysis was performed on the ash from the fully burned GR2.9 and GR3.9 demineralized kerogen. Figures 11 and 12 show the spectra from this analysis and Table 1 shows the quantitative analysis. As expected, the ash from both samples is high in iron and sulfur, as well as calcium. The iron peak is particularly high in the GR3.9 sample, suggesting that pyrite was not eliminated from the sample during the demineralization process.



Figure 11: SEM/EDAX analysis of ash from the demineralized GR2.9 sample.



Figure 12: SEM/EDAX analysis of ash from the demineralized GR3.9 sample.

Element	<b>GR2.9</b> Wt	GR3.9 Wt
	%	%
0 K	31.47	26.02
NaK	0.49	0.31
MgK	2.23	2.20
AlK	2.72	2.62
SiK	0.62	0.67
P K	0.11	0.16
S K	9.32	3.20
K K	0.22	0.56
СаК	12.66	3.41
TiK	1.50	3.19
FeK	38.66	57.67
Total	100.00	100.00

Table 1. SEM/EDAX analysis of the GR2.9 and GR3.9 samples.

After tars were collected on glass wool packed into the cooled condensers, minimal amounts of dichloromethane were used to dissolve condensed tars for testing. Standard dichloromethane was used to prepare samples for analysis in the GC/MS. Deuterated dichloromethane was used to dissolve tar samples to be analyzed using NMR spectroscopy.

TGA experiments were conducted on demineralized GR-1, GR-2, and GR-3 kerogen samples at three different heating rates: 5°C/min, 10°C/min and 20°C/min. The objective of these tests is to

construct the kinetic model for isolated kerogen decomposition. The results are summarized in Table 2 and the thermograms are shown in Figure 13. The results showed that the thermal decomposition of the kerogens extracted from different oil shales followed the same onset points at specific heating rates. The onset points shifted to higher temperatures with increasing heating rate. A similar trend was observed during the decomposition of the organic matter from oil shale.

**Table 2**. TGA results from kerogen pyrolysis at three heating rates (5°C/min, 10°C/min and 20°C/min) followed by combustion (10°C/min).

Heating Rate	Sample ID	Initial mass, mg	Pyrolysis end T	Pyrolysis Wt. loss %	Coke %
	GR1-Kerogen-5°C_min	8.41	505°C	80.77	12.78
5°C/min	GR2-Kerogen-5°C_min	2.99	505°C	85.68	12.80
	GR3-Kerogen-5°C_min	5.67	507°C	74.57	12.37
	GR1-Kerogen-10°C_min	4.32	514°C	70.58	15.57
10°C/min	GR2-Kerogen-10°C_min	2.3	513°C	80.81	11.98
	GR3-Kerogen-10°C_min	6.77	515°C	67.58	10.92
	GR1-Kerogen-20°C_min	7.12	538°C	81.2	12.15
20°C/min	GR2-Kerogen-20°C_min	4.08	540°C	66.05	12.78
	GR3-Kerogen-20°C_min	6.75	540°C	76.06	13.33



**Figure 13**: Pyrolysis of GR kerogens at heating rates of 5°C/min, 10°C/min and 20°C/min. (a) GR-1 kerogen, (b) GR-2 kerogen and (c) GR-3 kerogen. Pyrolysis was followed by combustion at 10°C/min.

During the next quarter, the research team will fix the high pressure TGA and duplicate experiments will be run. Analysis of the TGA data will then be completed to give rate constants for one-step and distributed activation energy models. Team members will also complete the pyrolysis experiments on sample GR3.9 of the demineralized kerogen using the kerogen retort. If time permits, sample GR2.9 will also be completed. Finally, the will also work on the CPD version of the kerogen pyrolysis model. CPD is an engineering model based on chemical structure that describes pyrolysis.

#### Subtask 4.4 - Effect of Oil Shale Processing on Water Compositions (PI: Milind Deo)

This project has been completed.

#### Subtask 4.5 - In Situ Pore Physics (PI: Jan Miller, Chen-Luh Lin)

The Subtask 4.5 team completed a milestone to calculate directional (anistropic) permeability of the GR-1b and GR-1c kerogen-rich cores after pyrolysis at different reaction temperatures (425°C and 500°C) and a heating rate of 100°C/min based on pore network structure from X-ray computed tomography (CT) analysis coupled with Lattice-Boltzmann (LB) simulation. In addition, characterization of the texture change during pyrolysis was analyzed based on comparison of the same sections of GR-1b and GR-1c cores before and after pyrolysis.

Research on pore scale transport processes in the pyrolysis of oil sand and oil shale involves 3D multiscale X-ray CT analysis coupled with LB simulation. Previously, Subtask 4.5 researchers obtained three Skyline 16 oil shale cores (6" long, 1" in diameter), located from 461.2-461.7' (GR-1), 485.9-486.4' (GR-2), and 548.2-548.7' (GR-3) from Subtask 4.3 and scanned the full-length cores in sections before pyrolysis. To investigate the effect of reaction temperature, each core (GR-1, GR-2, GR-3) was cut into three sections (2" long, 1" in diameter) and each section was pyrolyzed by Sutask 4.3 researchers at the temperatures/conditions summarized in Table 3. After pyrolysis, selected pieces of these nine samples were scanned.

Sample No.	Initial Weight (g)	Reaction Temperature (°C)	Drill Hole Position for Thermocouple Wire
GR-1a	40.3217	350	Тор
GR-1b	40.4917	425	Bottom
GR-1c	41.6266	500	Bottom
GR-2a	61.8151	425	Тор
GR-2b	52.9283	500	Тор
GR-2c	50.7762	325	Тор
GR-3a	51.1995	500	Тор
GR-3b	51.7524	350	Тор
GR-3c	47.8818	425	Bottom

Table 3. Pyrolyzed oil shale samples examined at three different reaction temperatures.

Figure 14 shows the tri-planar image for GR-1b (pyrolysis temperature = 425°C, heating rate = 100°C/min) indicating the pore generation that occurs along the kerogen-rich layers during pyrolysis. Characterization of the texture change during pyrolysis is analyzed based on a comparison of the same sections of cores before and after pyrolysis. Based on the relative position of mineral grains inside the GR-1b, as shown in Figure 15, three slice pairs from the 3D images were identified at the same positions along the core before and after pyrolysis at 425°C. Before pyrolysis, the distance between the top (747) and bottom (698) layers is 49 voxels or 2041.83 µm (voxel resolution=41.67 µm). After pyrolysis, the distance between the top (278) and bottom (222) layers is 56 voxels or 2333.52 µm (voxel resolution=41.67 µm). Due to creation of pores during pyrolysis, the thickness of the core increases by 291.69 µm from 2041.83 µm to 2333.52 µm or 14.3% in porosity.



**Figure 14**: Tri-planar image of GR-1b (pyrolysis temperature = 425°C, heating rate = 100°C/ min).



**Figure 15**: Three slice pairs from 3D CT images identified at the same positions along the core before and after pyrolysis at 425°C with a heating rate of 100°C/min.

The absolute permeability is determined based on coupling with LB simulation using the HRXMT data subset for regions containing more cracks from GR-1b. Figure 16 shows the 3D views of LB simulated flow along the x-axis through the reconstructed high resolution X-ray microtomography (HRXMT) image of GR-1b samples. Once the solid phases are removed, the right-hand side of Figure 16 shows the nature of the flow channels. The velocity scale is color-coded as shown by the color bar in Figure 16. The estimated permeability after pyrolysis at 425°C is about 2.88x10<sup>-5</sup> cm<sup>2</sup> or 2919 darcy.



**Figure 16**: 3D views of LB simulated flow along x-axis through the reconstructed HRXMT image of GR-1b samples after pyrolysis (pyrolysis temperature = 425°C, heating rate = 100°C/min). The transparent solid phase on the right-hand side reveal the pore network structure after pyrolysis.

Similarly, Figure 17 shows the tri-planar image for GR-1c (pyrolysis temperature =  $500^{\circ}$ C, heating rate =  $100^{\circ}$ C/min). Based on the relative position of mineral grains inside GR-1c, as shown in Figure 18, two slice pairs from the 3D images were identified at the same positions along the core before and after pyrolysis at  $500^{\circ}$ C. Before pyrolysis, the distance between the top (235) and bottom (227) layers is 8 voxels or  $333.36 \,\mu$ m (voxel resolution 41.67  $\mu$ m). After pyrolysis, the distance between the top (143) and bottom (123) layers is 20 voxels or  $833.4 \,\mu$ m (voxel resolution 41.67  $\mu$ m). Due to creation of pores during pyrolysis, the thickness of the core increases by 500.04  $\mu$ m from 333.86  $\mu$ m to 833.4  $\mu$ m.



**Figure 17**: Tri-planar image of GR-1c (pyrolysis temperature = 500°C, heating rate = 100°C/ min).



**Figure 18**: Two slice pairs from 3D CT images identified at the same positions along the core before and after pyrolysis at 500°C with a heating rate of 100°C/min.

The absolute permeability is determined based on coupling with LB simulation using the HRXMT data subset for regions containing more cracks from GR-1c. Figure 19 shows the 3D views of LB simulated flow along the x-axis through the reconstructed HRXMT image of GR-1c samples. Once the solid phases are removed, the right-hand side of Figure 19 shows the nature of the flow channels. The velocity scale is color-coded as shown by the color bar in Figure 19. The estimated permeability after pyrolysis at 500°C is about 1.71x10<sup>-6</sup> cm<sup>2</sup> or 173 darcy.



Estimated Permeability = 1.71x10<sup>-6</sup> cm<sup>-2</sup> = 173 darcy

**Figure 19**: 3D views of LB simulated flow along x-axis through the reconstructed HRXMT image of GR-1c samples after pyrolysis (pyrolysis temperature = 500°C, heating rate = 100°C/min). The transparent solid phase on the right-hand side reveal the pore network structure after pyrolysis.

# Subtask 4.6 - Atomistic Modeling of Oil Shale Kerogens and Oil Sand Asphaltenes (PI: Julio Facelli)

In this quarter, the subtask deliverable to submit a paper to a journal that describes development & validation of 3D asphaltene and kerogen models was completed. The paper entitled "Modeling of Asphaltenes: Assessment of Sensitivity of <sup>13</sup>C SSNMR to Molecular Structure" by Badu, Pimienta, Orendt, Facelli and Pugmire was accepted for publication in the journal *Energy & Fuels.* An additional paper on kerogen modeling will be forthcoming, but data obtained on a trip to Argonne National Laboratory (ANL) by Anita Orendt in February 2012 is still being analyzed. Also in this quarter, the project team modeled the interaction of kerogen with mineral matrices, using fragments of published crystal structures of illite, dolomite and calcite. The calculations were completed at the molecular mechanic level of theory using the UFF potential available in Gaussian 09.

To model kerogen/mineral interactions, the Subtask 4.6 team studied the change in the energy of the system as a function of the distance between the kerogen and the mineral. Only single point energies were calculated for each separation; the kerogen was not allowed to change its geometry. The model used and the results for illite are shown in Figures 20 and 21, respectively; the corresponding models and results for calcite are shown in Figures 22 and 23 and for

dolomite are shown in Figures 24 and 25. The plots of the energy versus distance between the kerogen and the mineral matrix indicate a local minimum of energy in all three cases. However, the quantitative analysis of the energy of interaction presented in Table 4 shows that there is no binding between the kerogen and mineral, at least not at this level of theory and with the chosen models. In this table,

Energy of Interaction = 
$$E(a,b)$$
-  $E(a)$ - $E(b)$  (3)

where E(a) is the energy of the kerogen, E(b) is the energy of mineral matrix, and E(a,b) is the energy of the kerogen/mineral system.



Figure 20 (left): Model used in calculation of interaction energy between kerogen and illite.

**Figure 21 (right**): UFF energy of the kerogen\_illite system as a function of the distance between the kerogen and illite units.



Figure 22 (left): Model used in calculation of interaction energy between kerogen and calcite.

**Figure 23 (right)**: UFF energy of kerogen\_calcite system as a function of the distance between the kerogen and calcite units.



Figure 24 (left): Model used in the calculation of the interaction energy between kerogen and dolomite.

**Figure 25 (right)**: UFF energy of the kerogen\_dolomite system as a function of the distance between the kerogen and dolomite units.

**Table 1**. Energy of interaction for the kerogen/mineral system.

	Energy of Interaction (Kcal/mol)*						
Distance (Å)	illite	calcite	dolomite				
2.30	129.46	27.55	79.29				

2.50	54.11	20.91	58.10
2.75	33.71	20.76	48.95
3.00	32.00	23.10	47.58
3.25	34.33	25.81	48.92
3.50	37.43	28.34	51.04
3.75	39.41	30.56	53.23
4.00	43.16	32.47	55.25

The face of the mineral matrix on which the kerogen is placed was chosen by considering the uniformity of atoms present in the contact plane and the size of the cluster in mind. In the illite case, this face is defined by the *b* and *c* crystallographic axes with the thickness of the mineral unit along the *a* axis; this face was chosen as it is parallel to the layered structure of the material. Calculations were also completed with the kerogen placed against the other two surfaces (i.e., mineral units having the thickness along the *b* and *c* crystallographic axis, respectively); binding was not found in either of these two additional orientations. For calcite and dolomite, the crystallographic axes *a* and *b* are equal. The model used to obtain the results presented in the table was with the face being the plane defined by the *b* and *c* crystallographic axes and the thickness along *a* crystallographic axis. Similar calculations have been performed for the interaction of kerogen on calcite and dolomite crystals with thickness taken along the unique *c* axis. Again, binding was not indicated by the calculations performed.

Further calculations are being completed using semi-empirical methods to see if the results are a function of the method used. In addition, calculations in which the kerogen geometry is allowed to vary are being completed to see if these will result in a binding interaction.

#### Subtask 4.7 - Geomechanical Reservoir State (PI: John McLennan)

The milestone to complete the experimental matrix has been delayed. In hindsight, the initial plan for testing was unrealistic. Difficulties in completing fabrication were not anticipated. The project team decided to switch machine shops because of poor turnaround and have seen improved response times with the new machine shop. Team members are coordinating with work being done on coal in the same apparatus and will carry out unconfined, ambient and heated testing outside of the vessel in the May-June time frame.

The project team did complete several design modifications and added capabilities to the apparatus in this quarter as listed below:

- The end cap fixtures have been modified and machining has been completed.
- Modifications to the clamshell heaters are being made to ensure that they seat properly around the sample. These are in-house. Team members will be testing them out outside of the vessel in an unconfined environment in May.
- Fixtures for the linear variable differential transducers (LVDT) are being designed.
   Originally, the displacement of the pump piston was going to be used to measure axial displacement, but this method is not accurate enough and LVDTs will be used instead.
- Complications in applying axial stress are being debugged. While the piston system is excellent, the pump, which is external to the vessel, has inadequate sensitivity.
- The LabView<sup>™</sup> interface that will be used to record data during the tests is being programmed.
- Permeability and porosity of the oil shale samples that will be used in the in-situ testing simulation were performed gratis by TerraTek, a Schlumberger Company. The tests

entailed crushed porosity and permeability measurements and pulse decay permeability measurements on uncrushed, plug samples.

## Subtask 4.8 - Developing a Predictive Geologic Model of the Green River Oil Shale, Uinta Basin (PI: Lauren Birgenheier)

The Subtask 4.8 team re-ran samples from the Skyline 16 core using QEMscan analysis with improved mineral definitions. The results have been compiled into a presentation that is attached as Appendix B. Also in this quarter, elemental X-ray fluorescence analysis was collected on the Asphalt Wash 1 core. The data have been calibrated for mudstones and are now being plotted and evaluated. Plans for next quarter include a description of one additional Green River core (SUB-12) at the Utah Geological Survey.

#### Subtask 4.9 - Experimental Characterization of Oil Shales and Kerogens (PI: Ronald Pugmire)

During this quarter, the milestone to characterize the bitumen and kerogen from three Skyline 16 core segments (GR-1, GR-2, and GR-3) was completed. The data set includes <sup>13</sup>C solution NMR data on the bitumen and <sup>13</sup>C solid state nuclear magnetic resonance (NMR), small angle x-ray scattering (SAXS) and atomic pairwise distribution functions (PDF) data on the kerogen isolated from GR-1, GR-2, and GR-3; however, analysis of all the data is still being completed. The solid state <sup>13</sup>C NMR on the kerogen from the three segments was completed last quarter and presented in the last quarterly report. Additionally, the research team focused its NMR efforts on the analysis of the char and tar samples from the pyrolysis experiments performed by Professor Tom Fletcher as part of Subtask 4.3.

Subtask 4.9 researchers isolated and analyzed a new sample of the GR-2 bitumen along with the bitumen samples from GR-1 and GR-3. All of the samples show substantially the same <sup>13</sup>C resonances with small differences in intensity, likely within experimental error. The fraction of aromatic carbons measured 10.9%, 9.9%, and 7.7% for bitumen isolated from GR-1, GR-2, and GR-3, respectively. Note that the result for the new sample of bitumen from GR-2 is somewhat higher than reported for the previous sample (6.0%) in last quarter's report. The older sample is believed to be less pure than the new one; thus, the new results are considered to be more reliable. It should be noted that the signal-to-noise in the aromatic region of the spectra is quite low, and the results given above should be interpreted to mean that the aromatic content of the three bitumen samples is essentially the same. However, the aromatic content of the bitumen is substantially lower than that of the kerogen from these cores.

Using a modification of the DEPT experiment, it is possible to produce quantitative carbon spectra for all protonated carbons. Thus, even though the bands overlap, it is possible to separate protonated from non-protonated carbons in the aromatic region by comparing standard NOE suppressed quantitative carbon data with the modified DEPT data. For the GR-1 and GR-2 bitumen samples, this treatment yields 40% and 50% of the aromatic carbons as protonated carbons, respectively. Thus, about half of the aromatic carbons are non-protonated, consisting of both substituted and bridgehead carbons. Analogous data is being acquired for the GR-3 bitumen and will be reported later.

The trip to the Advanced Photon Source (APS) at ANL on February 11-17, 2012, allowed for the acquisition of SAXS and PDF measurements on both the ground shale and the kerogen samples from all three segments (GR-1, GR-2, GR-3) of the Skyline 16 core. This data will be added to the SAXS data on the whole rock shale obtained in a previous visit (March 2011) to the APS. SAXS measurements were also completed on the GR-2 kerogen with CO<sub>2</sub> loading under

pressure. Processing and analysis of this data is ongoing and will be reported on in the next quarterly report.

Preliminary results from the NMR analysis of tars obtained from the pyrolysis of GR-1, GR-2, and GR-3 kerogens indicate that the tars vary quantitatively but not qualitatively as a function of pyrolysis temperature. The few samples generated thus far show essentially the same carbon resonances, but the ratios of the major components vary somewhat. More detailed results will be forthcoming as complete temperature profiles are completed.

During this quarter, solid state NMR analysis was done on several chars produced by pyrolysis of the three kerogen samples. The samples are identified by the kerogen used and the temperature at which the pyrolysis was stopped. The samples which were analyzed were: the GR-1 kerogen chars produced at temperatures of 300°C, 375°C and 410°C; a GR-3 kerogen char produced at 434°C; and GR-2 kerogen chars produced at 375°C, 425°C and 525°C.

Spectra from the original GR-2 oil shale, the kerogen isolated from this shale, and the chars produced from the pyrolysis of this kerogen are shown in Figure 26. Of the three oil shales being studied, GR-2 has the least amount of ferri/ferro-magnetic material in the sample. Neither the spectra of the kerogen nor of the 375°C char have aliphatic sidebands, indicating that there is no ferri/ferro-magnetic material in the sample. However, the spectrum of the 425°C char has aliphatic sidebands, probably due to some mineral matter transformation. In this 425°C char the aromaticity increased to 0.35 from 0.18 in the kerogen as aliphatic material is lost during heating. The average aliphatic chain length decreased from about 13 carbons to about 6 carbons. The 525°C sample is totally aromatic with very large aromatic sidebands; this level of carbonization is much greater than any other Green River kerogen samples previously analyzed at these temperatures in this laboratory. These differences in carbonization may be a function of the differences in the type of mineral matter.



Figure 26: The original GR-2 oil shale, the kerogen isolated from this shale, and chars obtained from the pyrolysis of this kerogen. The aliphatic sideband (indicated by the yellow line), present

in the shale but not in the kerogen nor the 375°C char, returns in the 425°C char as mineral matter that has reacted. At 525°C, only aromatic carbon is left.

Dipolar dephased spectra (showing only nonprotonated and mobile carbons) of the three chars made from the GR-1 kerogen sample are shown in Figure 27 along with the spectrum of the original kerogen. Very little change, outside of experimental error, can be seen, even for highest temperature (410°C) char. The one clear change in the samples is a monotonic decrease in the peak (yellow line) corresponding to carboxyl groups; this signal is mostly due to acids as the methoxy peak at about 52 ppm, indicative of esters, is very small even in the original kerogen. This peak can be large when methyl esters are formed from methanol during demineralization. The decrease in this carboxyl peak should correspond to the release of CO<sub>2</sub> during the early stages of pyrolysis before much tar is released.



**Figure 27:** Dipolar dephased spectra of GR-1 kerogen and three chars obtained from the pyrolysis of this kerogen. Only nonprotonated carbons, methyls and mobile protonated carbons remain. The main change with temperature is the loss of carboxyl groups (yellow line) along with a little rearrangement of aromatic bands.

#### Task 5.0 - Environmental, Legal, Economic and Policy Framework

<u>Subtask 5.1 – Models for Addressing Cross-Jurisdictional Resource Management (PI: Robert Keiter, John Ruple)</u>

Subtask 5.1 researchers completed and submitted the final topical report to Robert Vagnetti. The other deliverable for this project, the submission of an article for publication in a law review addressing issues pertaining to conjunctive water management, was completed in early 2011 with the publication of "Clear Law and Murky Facts: Utah's Approach to Conjunctive Surface and Groundwater Management" in the Idaho Law Review. A preprint of this article is available on the ICSE website.

Subtask 5.2 - Conjunctive Management of Surface and Groundwater Resources (PI: Robert Keiter, John Ruple)

This quarter, Subtask 5.2 researchers edited and resubmitted the final topical report in accordance with the comments received from Robert Vagnetti.

#### <u>Subtask 5.3 - Police and Economic Issues Associated with Using Simulation to Assess</u> <u>Environmental Impacts (PI: Robert Keiter, Kirsten Uchitel)</u>

Research efforts this quarter continued to focus on gathering material relevant to surveying the legal standards articulated in judicial opinions addressing the role and value of modeling in assessing environmental risks or harms.

#### 6.0 – Economic and Policy Assessment of Domestic Unconventional Fuels Industry

#### Subtask 6.1 Engineering Process Models for Economic Impact Analysis (PI: Terry Ring)

Process models for ex situ oil shale production and ex situ oil sands production were completed in this quarter and have been incorporated into Subtask 6.3. Work next quarter will focus on finalizing the two in situ production process, one for oil shale and one for oil sands. The milestone to provide models used and data collected to the ICSE repository and the deliverable to provide a topical report describing the process models used and a summary of parameters analyzed are both delayed until Subtask 6.3 is completed. These delays have occurred because the PI on this project accepted a part-time job with a private company and a key graduate student defended his thesis and left the university.

#### Subtask 6.2 - Policy analysis of the Canadian oil sands experience (PI: Kirsten Uchitel)

The topical report being prepared for this Subtask was delayed due to continuing revisions and drafting required both by reviewer comments and by the need for analytic consistency between the economic analysis of oil sands presented in the topical report for this Subtask and the Market Assessment report. Substantial work was begun on needed updates to the policy analysis and discussion portions of the topical report. Completion of the topical report for this Subtask is anticipated during the next quarter provided that finalization of the economic and policy pieces of the Assessment proceeds on schedule.

#### Subtask 6.3 - Market Assessment Report (PI: Jennifer Spinti)

Page layout on Sections 1-6 (introduction, unconventional liquid fuel resources, fiscal policy, externalities, description of methodology, ex situ oil shale scenario) is complete and Section 8 (ex situ oil sands scenario) is currently in the layout process. Copies of these sections are available upon request. Team members are planning to finalize Section 7 (in situ oil shale), 9 (in situ oil sands), and 10 (macroeconomic analysis of both ex situ development scenarios) in the next quarter.

#### 7.0 – Strategic Alliance Reserve

The Task 7.0 project team has regularly scheduled meetings with its industrial partner AMSO to share information and research results and to determine research direction. Meetings during this quarter were held on January 27 and March 8 on the University of Utah campus. The team

also prepares and circulates a biweekly report that provides an update on recent activities and results.

#### Subtask 7.1 – Geomechanical Model (PI: John McLennan)

No report received.

#### Subtask 7.2 – Kinetic Compositional Models and Thermal Reservoir Simulators (PI: Milind Deo)

Because geomechanics has significant impact on reservoir simulation, the Subtask 7.2 project team has integrated a geomechanical model into a K-value-based thermal reservoir model in the Advanced Reactive Transport Simulator (ARTS) developed at the University of Utah. A linear thermal poroelasticity stress constitutive law is used:

$$\sigma = \sigma' - \alpha P - 3\beta K_b T \tag{4}$$

where  $\sigma'$  is the effective stress,  $\alpha$  is the Boit coefficient,  $\beta$  is the linear thermal expansion coefficient,  $K_b$  is the bulk modulus, and P and T are the pore pressure and temperature in the reservoir.

In the ARTS framework, the K-value-based thermal reservoir model and a geomechanical model with the thermal stress constitutive relationship shown in Equation (4) are coupled to perform the reservoir simulation of a thermal recovery process with coupled geomechanics. An iterative coupling scheme is used; the coupling process is shown in Figure 28. The thermal reservoir model and geomechanical model are both initialized at the beginning of the simulation. The temperature and pressure in the geomechanical model are updated by the thermal reservoir model, and the porosity and permeability in the thermal reservoir model are updated by the geomechanical model. With the updated information, the whole system is solved to convergence through nonlinear and linear solver loops.



Figure 28: Geomechanical coupling process in ARTS with thermal stress model.

ARTS has the capability of modeling complex fracture networks through the Discrete Fracture Network (DFN) model, and this is also coupled with geomechanics. Indeed, the thermal model implemented in ARTS can model the complex kinetics involved during the thermal recovery process. Results of a simple demonstration case to show the capability of geomechanical coupling with thermal stress will be provided in the next quarterly report.

#### Subtask 7.3 - Rubblized Bed High Performance Computing Simulations (PI: Philip Smith)

In the past quarter, the Subtask 7.3 project team has begun quantifying the effects of convective channels on thermal history and temperature distribution inside a representative oil shale bed geometry. They have constructed a series of simplified computational domains with varying crack sizes and started to run simulations using their operator-splitting algorithm developed for long-term heating tests. They have also created geometric representations and simulations of the process used by AMSO. Through the work, team members continue to explore the capabilities of Star-CCM+, a commercial software package the project team is using to develop an HPC CFD-based simulation tool to study underground thermal heating of oil shale.

This subtask builds on work previously completed as part of Phase I of Subtask 4.1. That work includes the development of a rubblized shale geometry and the use of DEM capabilities in Star-CCM+ to create the representative fractured pieces of shale. During this quarter, team members have begun to study and quantify the effects of convective channels on the thermal distribution and thermal history of pieces of shale within the representative computational geometry (a 1 m x 1 m domain). For this study, the sizes of convective channels were varied from 5 mm to 15 mm. For comparison purposes, geometries have also been constructed using

a solid block of shale (effective crack size of 0 mm) and an empty computational domain (infinitely large crack size). Three temperature probes are included within each computational domain, as well as a volume-averaged temperature monitor. The project team plans to compare the temperature distributions as a function of time for all of the geometric domains. All five computational geometries with the respective temperature probe locations are shown in Figure 29.



**Figure 29**: Computational geometries used to quantify the effect of varying crack size on the thermal history of oil shale pieces.

For all simulations, the bottom boundary condition serves as the heating source with a constant temperature of 700 K, while all other sides remained insulated. During this quarter, only one computation from the suite of these simulations was completed. The temperature results for the computation with crack size of 15 mm are shown in Figure 30. The temperature captured by probe 3 (probe closest to the heating element) shows the earliest and fastest heating rate when compared to the other two probes. However, probe 1 (the probe furthest away from the heating element – close to the top of the domain) displays the second highest temperature among the three probes, illustrating how the convective channels allow the heat to rise to the upper part of the domain and thus increase the effective heating inside the computational domain. The effect of convective heating is further illustrated in Figure 31, where the entire domain is seen to be heating more-or-less uniformly, indicating the importance of the convective channels within the shale bed geometry. This temperature distribution resulting from convection is in contrast to the conductive mode of temperature distribution, which decreases with increasing distance from the heat source. In the next quarter, the project team plans to complete this study and to quantify the effects of crack size on the thermal history of the pieces of shale at specified locations.



Figure 30: Thermal history plots for domain with crack size of 15 mm.



**Figure 31**: Convective heat transfer inside the computational geometry with crack size of 15 mm.

The Subtask 7.2 team has also created a computational domain of the actual AMSO heater test experiment and implemented directional properties of the oil shale provided by AMSO. The computational domain is shown in Figure 32. Team members are collaborating very closely with AMSO scientists and receive weekly updates with the latest results of the heater test. As a result, this simulation will provide a very close representation of the actual AMSO experiment and will help AMSO scientists evaluate and better understand their experimental process.



Figure 32: Computational representation of the AMSO process.

#### CONCLUSIONS

One subtasks were completed during this quarter, Subtask 5.2 (Conjunctive Management of Surface and Groundwater Resources). The topical report has been submitted to DOE and will be revised as necessary based on any feedback that is received. Subtask 4.6 (Atomistic Modeling of Oil Shale Kerogens and Oil Sand Asphaltenes) will be completed next quarter when a second paper on kerogen modeling is submitted. The seven completed sections of the Market Assessment are available for review upon request.

#### **COST PLAN/STATUS**

	Yr. 1								Yr. 2			
Papalina Paparting Quarter BHASE I	Q	1	C	2		Q3	Q4		Q5		Q6	
Baseline Reporting Quarter - PTIAGE T	7/1/09 - 1	2/31/09	1/1/10 -	3/31/10	4/1/10	4/1/10 - 6/30/10		9/30/10	10/1/10 - 12/31/10		1/1/11 - 3/31/11	
	Q1	Total	Q2	Total	Q3	Total	Q4	Total	Q5	Total	Q6	Total
Baseline Cost Plan												
Federal Share	484,728	484,728	484,728	969,456	484,728	1,454,184	484,726	1,938,910	323,403	2,262,313	798,328	3,060,641
Non-Federal Share	121,252	121,252	121,252	242,504	121,252	363,756	121,254	485,010	80,835	565,845	199,564	765,409
Total Planned	605,980	605,980	605,980	1,211,960	605,980	1,817,940	605,980	2,423,920	404,238	2,828,158	997,892	3,826,050
Actual Incurred Cost												
Federal Share	420,153	420,153	331,481	751,634	547,545	1,299,179	428,937	1,728,116	593,386	2,321,502	307,768	2,629,270
Non-Federal Share	29,456	29,456	131,875	161,332	151,972	313,304	100,629	413,933	191,601	605,534	45,101	650,635
Total Incurred Costs	449,609	449,609	463,356	912,966	699,517	1,612,483	529,566	2,142,049	784,987	2,927,036	352,869	3,279,905
Variance												
Federal Share	64,575	64,575	153,247	217,822	-62,817	155,005	55,789	210,794	-269,983	-59,189	490,560	431,371
Non-Federal Share	91,796	91,796	-10,623	81,172	-30,720	50,452	20,625	71,077	-110,766	-39,689	154,463	114,774
Total Variance	156,371	156,371	142,624	298,994	-93,537	205,457	76,414	281,871	-380,749	-98,878	645,023	546,145

Note: Q5 and Q6 reflect both CDP 2009 and CDP 2010 SF424a projections as the award periods overlap.

	Yr. 2			Yr. 3									
Reading Reporting Quarter, RUASE II	Q7		C	18		Q9		Q10		Q11		Q12	
Baseline Reporting Quarter - PHASE II	04/01/11 -	06/30/11	07/01/11	- 09/30/11	10/01/11	- 12/31/11	01/1/12 -	03/31/12	04/01/12 - 06/30/12		07/01/12 - 09/30/12		
	Q7	Total	Q8	Total	Q9	Total	Q10	Total	Q11	Total	Q12	Total	
Baseline Cost Plan													
Federal Share	712,385	3,773,026	627,423	4,400,449	147,451	4,547,900	147,451	4,695,351	147,451	4,842,802	245,447	5,088,249	
Non-Federal Share	178,100	943,509	156,854	1,100,363	36,863	1,137,226	36,863	1,174,089	36,863	1,210,952	58,906	1,269,858	
Total Planned	890,485	4,716,535	784,277	5,500,812	184,314	5,685,126	184,314	5,869,440	184,314	6,053,754	304,353	6,358,107	
Actual Incurred Cost													
Federal Share	449,459	3,078,729	314,813	3,393,542	271,897	3,665,439	267,784	3,933,223		3,933,223		3,933,223	
Non-Federal Share	48,902	699,537	48,835	748,372	105,695	854,067	40,652	894,719		894,719		894,719	
Total Incurred Costs	498,361	3,778,266	363,648	4,141,914	377,592	4,519,506	308,437	4,827,943		4,827,943		4,827,943	
Variance													
Federal Share	262,926	694,297	312,610	1,006,907	-124,446	882,461	-120,333	762,128		909,579		1,155,026	
Non-Federal Share	129,198	243,972	108,019	351,991	-68,832	283,159	-3,789	279,370		316,233		375,139	
Total Variance	392,124	938,269	420,629	1,358,898	-193,278	1,165,620	-124,123	1,041,497		1,225,811		1,530,164	

	Yr. 4										
Develop Develop Orester DUAOF II	Q1	3	Q	Q14		Q15		Q16			
Baseline Reporting Quarter - FTIASE II	10/01/12 -	12/31/12	01/01/13	- 03/31/13	04/01/13 - 06/30/13		07/01/13 - 09/30/13				
	Q13	Total	Q14	Total	Q15	Total	Q16	Total		Total	Total
Baseline Cost Plan											
Federal Share	146,824	5,235,073	146,824	5,381,897	146,824	5,528,721	133,794	5,662,515			
Non-Federal Share	36,705	1,306,563	36,705	1,343,268	36,705	1,379,973	35,906	1,415,879			
Total Planned	183,529	6,541,636	183,529	6,725,165	183,529	6,908,694	169,700	7,078,394			
Actual Incurred Cost											
Federal Share		3,933,223		3,933,223		3,933,223		3,933,223			
Non-Federal Share		894,719		894,719		894,719		894,719			
Total Incurred Costs		4,827,943		4,827,943		4,827,943		4,827,943			
Variance											
Federal Share		1,301,850		1,448,674		1,595,498		1,729,292			
Non-Federal Share		411,844		448,549		485,254		521,160			
Total Variance		1,713,693		1,897,222		2,080,751		2,250,451			

#### **MILESTONE STATUS**

ID	Title/Description	Planned Completion Date	Actual Completion Date	Milestone Status
1.0	Project Management			
2.0	Technology Transfer and Outreach			
	Advisory board meeting	Jun-12		
	Hold final project review meeting in format determined jointly by DOE/NETL and ICSE	Jun-13		
3.0	Clean Oil Shale & Oil Sands Utilization with CO2 Management			
3.1	Lifecycle greenhouse gas analysis of conventional oil & gas development in the Uinta Basin			
	Complete modules in CLEAR <sub>uff</sub> for life-cycle CO2 emissions from conventional oil & gas development in the Uinta Basin	Jun-12		
3.2	Flameless oxy-gas process heaters for efficient CO2 capture			
	Preliminary report detailing results of skeletal validation/uncertainty quantification analysis of oxy-gas combustion system	Oct-11		Problems with CFD code will be addressed next quarter
3.3	Development of oil & gas production modules for CLEAR <sub>uff</sub>			
	Develop preliminary modules in CLEAR <sub>uff</sub> for conventional oil & gas development & produced water management in Uinta Basin	Oct-11	Dec-11	Discussed in Jan. 2012 quarterly report
3.4	V/UQ analysis of basin scale CLEAR <sub>uff</sub> assessment tool			
	Develop a first generation methodology for doing V/UQ analysis	Oct-11	Nov-11	Discussed in Jan. 2012 quarterly report
	Demonstrate full functionality (integration of all modules) of V/UQ methodology for conventional oil & gas development in Uinta Basin	Apr-12		Project on hold pending completion of Subtask 6.3
4.0	Liquid Fuel Production by In-Situ Thermal Processing of Oil Shale/Sands			
4.1	Development of CFD-based simulation tool for in-situ thermal processing of oil shale/ sands			

		Planned Completion	Actual Completion	Milestone
ID	Title/Description	Date	Date	Status
	Expand modeling to include reaction chemistry & study product yield as a function of operating conditions	Feb-12	Mar-12	Discussed in this quarterly report
4.2	Reservoir simulation of reactive transport processes			
	Incorporate kinetic & composition models into both commercial & new reactive transport models	Dec-11	Dec-11	Reported in Jan. 2012 quarterly report; additional information next quarter
	Complete examination of pore-level change models & their impact on production processes in both commercial & new reactive transport models	Jun-12		
4.3	Multiscale thermal processes			
	Complete thermogravimetric analyses experiments of oil shale utilizing fresh "standard" core	Sep-11	Sep-11	Discussed in Oct. 2011 quarterly report
	Complete core sample pyrolysis at various pressures & analyze product bulk properties & composition	Dec-11		Delayed until next quarter due to equipment problems
	Collection & chemical analysis of condensable pyrolysis products from demineralized kerogen	May-12		
	Complete model to account for heat & mass transfer effects in predicting product yields & compositions	Jun-12		
4.5	In situ pore physics			
	Complete pore network structures & permeability calculations of Skyline 16 core (directional/anisotropic, mineral zones) for various loading conditions, pyrolysis temperatures, & heating rates	Mar-12	Mar-12	Discussed in this quarterly report
4.6	Atomistic modeling of oil shale kerogens & oil sand asphaltenes			
	Complete web-based repository of 3D models of Uinta Basin kerogens, asphaltenes, & complete systems (organic & inorganic materials)	Dec-11	Dec-11	Discussed in Jan. 2012 quarterly report
4.7	Geomechanical reservoir state			
	Complete high-pressure, high-temperature vessel & ancillary flow system design & fabrication	Sep-11	Sep-11	Discussed in Oct. 2011 quarterly report
	Complete experimental matrix	Feb-12		Delayed due to equipment problems
	Complete thermophysical & geomechanical property data analysis & validation	Apr-12		

	Title/Description	Planned Completion	Actual Completion	Milestone
4.8	Developing a predictive geologic model of the Green River oil shale, Uinta Basin	Date	Date	Otatus
	Detailed sedimentologic & stratigraphic analysis of three cores &, if time permits, a fourth core	Dec-12		
	Detailed mineralogic & geochemical analysis of same cores	Dec-12		
4.9	Experimental characterization of oil shales & kerogens			
	Characterization of bitumen and kerogen samples from standard core	Jan-12	Jan-12	Email sent to R. Vagnetti
	Development of a structural model of kerogen & bitumen	Jun-12		
5.0	Environmental, legal, economic, & policy framework			
5.1	Models for addressing cross-jurisdictional resource management			
	Identify case studies for assessment of multi-jurisdictional resource management models & evaluation of utility of models in context of oil shale & sands development	Jun-11	Jul-11	Discussed in Oct. 2011 quarterly report
5.2	Conjunctive management of surface & groundwater resources			
	Complete research on conjunctive surface water & groundwater management in Utah, gaps in its regulation, & lessons that can be learned from existing conjunctive water management programs in other states	Aug-11	Aug-11	Discussed in Oct. 2011 quarterly report
5.3	Policy & economic issues associated with using simulation to assess environmental impacts			
	White paper describing existing judicial & agency approaches for estimating error in simulation methodologies used in context of environmental risk assessment and impacts analysis	Dec-12		
6.0	Economic & policy assessment of domestic unconventional fuels industry			
6.1	Engineering process models for economic impact analysis			
	Upload all models used & data collected to repository	Oct-11		Delayed by PI change, need to redo parts of analysis

ID	Title/Description	Planned Completion Date	Actual Completion Date	Milestone Status
7.0	Strategic Alliance Reserve			
	Conduct initial screening of proposed Strategic Alliance applications	Mar-11	Mar-11	
	Complete review and selection of Strategic Alliance applications	Jun-11	Jul-11	Discussed in Oct. 2011 quarterly report
	Implement new Strategic Alliance research tasks	Sep-11	Sep-11	Discussed in Oct. 2011 quarterly report
7.1	Geomechanical model			
	Infer permeability-porosity-temperature relationships, develop model that can be used by other subtasks	Dec-12		
	Make experimental recommendations	Aug-13		
7.2	Kinetic compositional models & thermal reservoir simulators			
	Incorporate chemical kinetics into thermal reservoir simulators	Jun-12		
	Demonstrate reservoir simulation of AMSO process	Sep-12		
	Incorporate poroelastic & geomechanical models into reservoir simulator	Jun-13		
7.3	Rubblized bed HPC simulations			
	Collect background knowledge from AMSO about characteristics & operation of heated wells	Jun-12		
	Perform generation 1 simulation - DEM, CFD & thermal analysis of characteristic section of AMSO rubblized bed	Sep-12		
	Perform generation 2 simulation that incorporates kinetic compositional models from subtask 7.2 and/or AMSO	Jun-13		

#### NOTEWORTHY ACCOMPLISHMENTS

The work performed by the Subtask 4.5 team that correlates textural change and its impact on permeability of oil shale core samples that have undergone pyrolysis under different reaction conditions (450°C and 500°C) is first of its kind. Additionally, the project teams that comprise Task 7.0 are pleased with the extent of interaction that has occurred with AMSO.

#### **PROBLEMS OR DELAYS**

Several project milestones and deliverables from Subtasks 3.1 (Phase I), 3.2, 3.3, 3.4, 6.1, and 6.2 continue to be delayed by work on the Market Assessment. The Market Assessment delays are due to the departure of a key graduate student and the unavailability of a PI who has accepted a part time position outside the university. Seven of the ten Market Assessment sections have been completed and prepared for publication. For Subtask 4.2, the milestone to incorporate advanced kinetic and composition models for oil shale pyrolysis into commercial and new compositional reservoir simulators has been developed in concept as reported last guarter. However, additional details about the new models will be provided next guarter. Due to equipment malfunctions with the TGA, Subtask 4.3 researchers were unable to collect pyrolysis kinetics data and to perform pressurized runs. Additional repair is needed before the pressurized runs can be completed. Subtask 4.5 researchers were unable to perform a permeability analysis of the reacted core after pyrolysis reactions under different loading conditions because the samples were not available from the Subtask 4.3 project team. An additional paper on the kerogen modeling was dependent on the timing of the trip to ANL to collect data. That trip occurred in February 2012 and the data is currently being analyzed so that the kerogen modeling paper can be completed. Finally, the Subtask 4.7 project team experienced extremely slow turnaround times with equipment fabrication that has significantly delayed their initial testing plan. After switching to a different machine shop, they have seen improved response times that will enable them to move forward with equipment debugging and initial experiments in this next quarter.

#### **RECENT AND UPCOMING PRESENTATIONS/PUBLICATIONS**

#### List of publications/presentations

- Ruple, J. (2011). Clear law and murky facts: Utah's approach to conjunctive surface and groundwater management. *Idaho Law Review, 47*, 217-254.
- Bauman, J. H., Bhide, R. & Deo, M. D. (2011, October). An evaluation of porosity and permeability changes in oil shale due to thermal stresses. Paper presented at the 31<sup>st</sup> Oil Shale Symposium, Colorado School of Mines, Golden, CO.
- Orendt, A., Facelli, J. C. & Pugmire, R. (2011, October). Atomistic modeling of oil shale kerogens and asphaltenes. Paper presented at the 31<sup>st</sup> Oil Shale Symposium, Colorado School of Mines, Golden, CO.
- Orendt, A., Pugmire, R., Facelli, J. C. & Birgenheier, L. (2011, October). Structural characterization of segments of a Green River oil shale core and the kerogen isolated from these segments. Paper presented at the 31<sup>st</sup> Oil Shale Symposium, Colorado School of Mines, Golden, CO.

- Orendt, A., Pugmire, R., Facelli, J. C. & Birgenheier, L. (2011, October). Detailed analytical data from select segments of a Green River oil shale core. Poster presented at the 31<sup>st</sup> Oil Shale Symposium, Colorado School of Mines, Golden, CO.
- Tran, T. Q., McLennan, J. D., Deo, M. &and Okerlund, R. (October, 2011). Evaluation of transport properties of in-situ processed oil shale. Poster presented at the 31<sup>st</sup> Oil Shale Symposium, Colorado School of Mines, Golden, CO.
- Vanden Berg, M. & Birgenheier, L. (2011, October). Not all rich zones are created equal: Geologic characterization results of Green River formation core descriptions from Utah's Uinta Basin, including the newly drilled Skyline 16 core. Paper presented at the 31<sup>st</sup> Oil Shale Symposium, Colorado School of Mines, Golden, CO.

Wilkey, J. (2011, December). Evaluation of the economic feasibility of heavy oil production processes for West Sak Field. MS Thesis, University of Utah, Salt Lake City, UT.

- R. Keiter, J. Ruple, H. Tanana and R. Holt. (2012, January). Conjunctive surface and groundwater management in Utah: Implications for oil shale and oil sands development. Submitted to the Department of Energy under DOE Award No. DE-FE0001243.
- Tiwari, P. & Deo, M. (2012, February). Detailed kinetic analysis of oil shale pyrolysis TGA data. *AICHE Journal*, *58*(2), 505-515.
- Spinti, J. (2012, February 15). Presenter/panelist *Oil sands: How Utah can improve on the Alberta model.* Utah Governor's Energy Development Summit, Salt Lake City, UT.
- Deo, M. (2012, February 15). Presenter/panelist *Oil sands: How Utah can improve on the Alberta model.* Utah Governor's Energy Development Summit, Salt Lake City, UT.
- Tiwari, P. & Deo, M. (2012, April). Compositional and kinetic analysis of oil shale pyrolysis using TGA-MS. *Fuel*, *94*, 333-341.
- Rosenberg, M., Birgenheier, L. & Vanden Berg, M. (2012, April) Outcrop examination and sequence stratigraphy of the lacustrine Green River Formation, Uinta Basin, Utah: Implications for conventional and unconventional oil and gas development. Poster presented at the annual meeting of the American Association of Petroleum Geologists Annual Convention, Long Beach, CA, April 22-25, 2012.
- Eby, D., Chidsey, T., Vanden Berg, M. & Laine, M. (2012, April). Microbial carbonates from core and outcrop, Tertiary (Eocene) Green River Formation, Uinta Basin, Utah. Paper to be presented at the annual meeting of the American Association of Petroleum Geologists.
- Badu, S., Pimienta, I. S. O., Orendt, A. M. Facelli, J. C. & Pugmire, R. J. (2012). Modeling of asphaltenes: Assessment of sensitivity of <sup>13</sup>C SSNMR to molecular structure. Submitted to *Energy & Fuels, 26(4),* 2161-2167.
- Fletcher, T. (2012, May 15). Kinetics of Uinta Basin oil shale pyrolysis. Presentation at the 2012 University of Utah Unconventional Fuels Conference, Salt Lake City, UT.
- Ruple, J. (2012, May 15). Wilderness quality lands and unconventional fuel development. Presentation at the 2012 University of Utah Unconventional Fuels Conference, Salt Lake City, UT.

- Bauman. J. H. & Deo, M. D. (n.d.) Simulation of a conceptualized combined pyrolysis, in situ combustion, and CO<sub>2</sub> storage strategy for fuel production from Green River oil shale. Submitted to *Energy and Fuels*.
- Pimienta, I. S. O., Orendt, A. M., Pugmire, R. J., Facelli, J. C., Locke, D. R., Winans, R. E., Chapman, K. W. & Chupas, P. J. (n.d.). Three-dimensional structure of the Siskin Green River oil shale kerogen model: A computational study. Manuscript in final draft form and will be submitted to a journal in May.
- Lin, C. L., Miller, Hsieh, C. H., Tiwari, P. & Deo, M. D. (n.d.). Pore scale analysis of oil shale pyrolysis by X-ray CT and LB simulation. Paper is being revised and will sent to a peer-reviewed journal.
- Orendt, A., Pimienta, I. S. O., Badu, S., Solum, M., Pugmire, R. J., Facelli, J. C., Locke, D. R., Winans, R. E., Chapman, K. W. & Chupas, P. J. (n.d.). Three-dimensional structure of the Siskin Green River oil shale kerogen model: A comparison between calculated and observed properties. Manuscript in draft form.

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Campbell, J. H., Koskinas, G. H., & Stout, N. D. (1978). Kinetics of oil generation from Colorado oil shale. *Fuel, 57*.

Coraggio, G. & Laiola, M. (2009). *Combustion of NG and pulverized coal in a mixture of oxygen and RFG* (IFRF. Doc. No F110/y/01). Pisa, Italy: International Flame Research Foundation.

Granoff, B. & Nuttall, H. E. (1977). Pyrolysis kinetics of oil-shale particles. Fuel, 56.

Sweeney, J. J., Burnham, A. K., & Braun, R. L. (1987). A model of hydrocarbon generation from type I kerogen: Application to Uinta Basin, Utah. *The American Association of Petroleum Geologists Bulletin*, *71(8)*.

#### APPENDIX A. 2011 ISCE Advisory Board Meeting: Summary of Board Recommendations

**Board Members in Attendance**: Ian Andrews, PacifiCorp Energy; Jim Holtkamp, Holland & Hart; Robert Lestz, GasFrac Energy Services; Dianne Nielson, Former Utah State Energy Advisor; Laura Nelson, Red Leaf Resources, Inc.; David Pershing, University of Utah; Mark Raymond, Uintah County Commission; Adel Sarofim, University of Utah

**Board Members Unable to Attend:** Spencer P. Eccles, Utah Governor's Office of Economic Development; Hishashi "Sho" Kobayashi, Praxair, Inc.; John Marion, Alstom Power; Madhava Syamlal, National Energy Technology Laboratory

#### **ICSE ADVISORY BOARD RECOMMENDATIONS – BACKGROUND**

The overarching issue discussed by the ICSE Advisory Board at its 2011 Annual Meeting was how ICSE should position itself for the 2013 termination of several years of Congressional earmark funding and research programming. The issue of ICSE's positioning was discussed at greatest length in the contexts of what role the Board can play in helping ICSE obtain funding, and what funding opportunities should be pursued. Additionally, funding was discussed in terms of selecting ICSE research focus areas going forward and whether to maintain ICSE's current multidisciplinarity. The specific questions used to guide the Advisory Board discussion were contained in the materials provided to Advisory Board members at the Annual Meeting and are attached to these recommendations.

#### ICSE Advisory Board Recommendations – Funding & The Role of the Board

The Board Members in attendance at the 2011 Annual Meeting uniformly expressed the sentiment that it was the role of the Board to aid ICSE in preserving its integrity as a multidisciplinary Institute (discussed in greater detail below) and ensuring financial support for ICSE research. Several Board Members articulated the need for the Board to provide assistance directed at maintaining ICSE's broad-based research objectives. To that end, Board Members identified several potential sources of funding and possible approaches to obtaining funding from those sources. Where individual Board Members offered to liaison between ICSE and specific individuals or entities during the discussion portion of the Board Meeting, it is so noted at the conclusion of the description of the particular funding source.

#### **ICSE ADVISORY BOARD RECOMMENDATIONS – SPECIFIC FUNDING OPPORTUNITIES**

The specific funding opportunities discussed at the 2011 Annual Meeting are enumerated below. The list begins with the State of Utah, which was identified as a promising source of potential funding, and is alphabetical thereafter.

#### The State of Utah

The State of Utah was suggested as a possible source of broad funding to replace a portion of the Congressional earmark funding set to expire at the close of the third quarter of 2013. It was proposed that ICSE hold meetings with members of the Utah State Legislature regarding the role ICSE might play in supporting the development of energy resources and policies in Utah. Roger Barrus (Utah House of Representatives) was suggested as the most promising contact for these discussions. It was noted that Representative Barrus has long advocated for Utah to pursue funding initiatives along the lines of Wyoming's Energy Producing States Coalition initiative (discussed further below), and that perhaps ICSE could play a role in such initiatives. It was proposed that ICSE develop a white paper presenting ICSE's capabilities and ability to

contribute to more efficient analysis of state research initiatives and energy policy questions to be circulated among the executive legislative leadership. It was noted that increasing efficiencies and recovering costs are important and appealing themes for the current political leadership. Board Members observed that having the state's political leadership view ICSE as a partner in advancing energy research and policy initiatives was key. Jim Holtkamp offered assistance as far as approaching Roger Barrus.

It was also suggested that ICSE hold meetings with the Utah Governor's Office in conjunction with steps taken to implement the Governor's Energy Plan. Lieutenant Governor Greg Bell was suggested as the best contact for such discussions. It was proposed that ICSE also submit the white paper described above to the Governor and Lieutenant Governor, along with appropriate members of their staffs.

Board Members also suggested that there might be specific research and funding opportunities connected to critical air quality issues in the Uinta Basin and related modeling needs.

<u>American Association of Petroleum Geologists (AAPG)</u> was suggested as a potential source of policy research funding through the Society of Petroleum Engineers (SPE). Robert Lestz offered assistance in inquiring to see how ICSE could best identify potential funding opportunities through SPE.

<u>American Petroleum Institute (API)</u> was suggested as a possible source for oil shale and oil sands research funding. Laura Nelson offered assistance in inquiring of Holly Hopkins at API to see how ICSE could best identify potential funding opportunities.

<u>Angel Investors</u> and similar venture capital groups that fund energy development. Jim Holtkamp expressed some familiarity with these groups through one of his partners at Holland & Hart. It was suggested that perhaps ICSE should find a means of presenting or otherwise reaching out to these groups.

<u>Department of Defense</u> was suggested as a possible source of funding. Al Walker of USTAR was suggested as a possible contact for identifying such projects and funding.

<u>Electric Power Research Institute (EPRI)</u> was suggested as a possible source of funding for clean coal research.

<u>Energy Producing States Coalition (EPSC)</u> was suggested as another possible funding source. The EPSC approach is favored by Roger Barrus (discussed above in the context of state funding opportunities), and seeks to maintain state authority over energy identities by building a common approach for new legislation across the member states, examining options for new legislation, and funding research. EPSC has a federal focus, based on effectively advancing the energy development priorities and interests of its founding member states (Alaska, Colorado, North Dakota, Utah, and Wyoming) and influencing federal regulation of the domestic energy resources portfolio. Laura Nelson offered assistance as far as approaching EPSC.

<u>Senator Mike Lee</u> was suggested as a potential source support of ICSE despite his stated objection to earmark funding. Mark Raymond noted that Senator Lee has reached out to the Uintah County community and expressed a desire to lead energy policymaking efforts originating in the Senate.

<u>Uintah County Energy Summit</u> was suggested as a source of networking and potential funding contacts. Mark Raymond offered assistance in reserving time for ICSE to present at the 2012 Summit.

<u>U.S. Carbon Sequestration Council</u> was suggested as a possible source of funding for carbon capture and sequestration research.

<u>Utah Science Technology and Research Initiative (USTAR)</u> was suggested as a potential partner and funding source for ICSE. In particular, the suggestion was made that ICSE approach Ted McAleer to see what role ICSE might play in USTAR's clean coal partnership efforts. Additionally, Board Members noted that USTAR is required to defend its budget every year, and thus might benefit from and be interested in broadening the scope of USTAR's energy focus and funding.

<u>Western Energy Alliance (WEA)</u> was suggested as a potential conduit for approaching industry for research funding, particularly in areas of present WEA focus, such as access and air quality. However, Board Members noted that WEA was currently in a state of transition. Mark Raymond offered assistance as far as approaching WEA when timely.

#### **ICSE** Advisory Board Recommendations – Research Focus Areas

ICSE Advisory Board Members uniformly recommended continued collaborative efforts with industry (along the lines of the demonstration scale projects endorsed by the Board at the 2010 Annual Board Meeting) as the preferred model for developing future ICSE research projects. Developing a partnership with policymakers, particularly at the Utah state government level, was also highly recommended. Exploring the possibility of multistate research initiatives along the lines of Patty Limerick's research projects through the Center of the American West at the University of Colorado Boulder, was also proposed. The Wallace Stegner Center at the University of Utah (whose Director, Bob Keiter, is a member of the ICSE Directorate) was suggested as a potential partner in any such efforts.

Continued or expanded coal research was noted by the Board Members to hold both potential promise and challenge as far developing collaborative projects with industry. Board Members saw promise in coal research stemming from both the significant coal resources available for development in Utah and Wyoming and the Governor's Energy Plan for the State of Utah making particular mention of continuing to utilize domestic coal for energy production. The challenge inherent in coal research identified by Board Members resulted from the predominance of anticipated reliance on natural gas over coal as far as future plans for electricity generation. Underground coal thermal treatment research was raised as an area of research potentially of interest to utilities if the research focused on technologies that provided the opportunity to use gas at its source without requiring major processing facilities. Clean coal technology was raised as an important area in which to continue and potentially broaden ICSE research efforts. Board Members expressed the sentiment that emerging areas of energy research and technology presented greater opportunities for industrial support.

Other conventional fossil fuels and transportation fuels were also noted as potential areas of research. It was suggested that ICSE might benefit from broadening into conventional petroleum, however, it was also noted that such action would likely be problematic from an internal University of Utah perspective given that such a focus would increase overlap between ICSE and the Energy and Geoscience Institute (EGI) at the University.

Several Board Members commented on the value of research focused on minimizing the environmental impacts of continued fossil fuel utilization and maximizing technological efficiencies, deeming these areas of research ideal for industrial collaboration and sharing research results with the broader community. Board Members also recommended continued research on technologies aimed at minimizing traditional criteria pollutants (ozone, particulate matter, carbon monoxide, nitrogen oxides, sulfur dioxide and lead), hazardous air pollutants (in anticipation of tightened MACT standards), and mercury.

A new area of activity suggested at the 2011 Board Meeting was for ICSE to develop a "tech services" role in providing educational services to industry, particularly in the areas of simulation science and verification, validation and uncertainty quantification (VVUQ). Developing such a program could offer ICSE another revenue source that also offered the benefit of broadening industrial awareness of ICSE's simulation science and VVUQ expertise and laying groundwork for networking and future funding opportunities. It was noted that the primary challenge associated with developing a tech services role for ICSE would be simultaneously accommodating shorter-term industrial and longer-term academic/student timeframes. Robert Lestz offered assistance in developing connections with industry for this purpose.

Another similar area of new activity suggested at the 2011 Annual Meeting was for ICSE to approach law firms based in Washington, D.C. that represent utility consortiums, such as the Utility Air Regulatory Group, in order to determine whether there might be an opportunity for ICSE to contract out its policy research services and products. The law firms of Baker & Botts LLP, Hunton & Williams LLP and Morgan, Lewis & Bockius LLP were specifically mentioned. Ian Andrews and Jim Holtkamp expressed familiarity with this network of consortiums and attorneys.

#### **ICSE ADVISORY BOARD RECOMMENDATIONS – MULTIDISCIPLINARITY**

The value of ICSE's current multidisciplinary research focus and faculty/staff/student makeup was submitted to the Board, specifically to address the question of whether ICSE should maintain a multidisciplinary identity in light of impending funding challenges. The Board was unanimous in its judgment that ICSE's multidisciplinary approach is "what really adds value" and termed the current Institute-wide identity and focus of ICSE as "critical to success." The Board Members uniformly viewed disaggregating ICSE and returning to loosely affiliated areas of individual research as detrimental to ICSE.

Speaking specifically to the policy component of ICSE's research focus, the Board urged ICSE to maintain its policy focus, and perhaps even use that policy focus to further distinguish itself from EGI, another University of Utah Institute engaged in fossil resource related research. It was suggested that ICSE should try to add a policy component to science-based research projects where possible.

Another observation made at the Board Meeting was that ICSE's policy focus, through either research or outreach events, might be a tool for identifying research and funding opportunities for ICSE by bridging otherwise unconsolidated industry views. It was suggested that ICSE try to communicate with industry members through their V.P.s of Public Affairs as possible funding sources for ICSE-sponsored public education and outreach events.

APPENDIX B. QEMSCAN Analysis of Green River Formation Oil Shale Samples, Skyline 16 Core, Eastern Uinta Basin, UT (see attached)

# QEMSCAN analysis of Green River Formation oil shale samples, Skyline 16 core, eastern Uinta Basin, UT

QEMSCAN = Quantitative Evaluation of Minerals by SCANning electron microscopy

Lauren Birgenheier Michael Vanden Berg James Taylor Green River Fm samples for QEMscan analysis from Skyline 16 core

						0259	11 12
Sample	Depth (ft)	Stratigraphic Source	Dominant mineralogy	Fischer Assay	Linholgie Units W Fachine	1 Resistring (chma) 1000	Caliper
GR-1	461.93- 462.92	Mahogany rich	Calcareous	~6o gal/ton	Subsc Zuer (94-108 f)		A Start
GR-2	485.9- 486.94	Mahogany lean	Calcareous	~28 gal/ton	tite tites {		4-2031 W ( Aug
GR-3	548.18- 549.15	Upper-R6	Dolomitic?	~22 gal/ton	GR4		All a Maria
GR-4	410.4- 410.5	R-8 rich	Calcareous	~23 gal/ton	GR1 GR2 Marchener		
GR-5	812.15- 812.3	R-5 rich	Dolomitic to clay-rich?	~26 gal/ton	GR3		



# Green River Qemscan Data

These analyses were completed at the Energy and Geoscience Institute at the University of Utah, on a QEMSCAN® 4300, which is built on a Zeiss Evo 50 SEM platform with four light element Bruker Xflash energy dispersive Xray detectors.

The QEMSCAN® was operated using an accelerating voltage of 20 kV and a specimen current of approximately 5 nA .

Species Identification Protocol (SIP) used for interpretation of the spectral data in this study was provided by FEI, O&G v3.3

iMeasure v.5.2 software was used for the data acquisition, and iDiscover v.5.2 for the spectral interpretation and data processing. All measurements were collected in field-scan mode, and X-ray data was collected every 10µm.

At 10 micron resolution, a 2mm X 2mm square has 40,000 pixels.



More info at http://www.reservoirs.earth.utah.edu/gemscan.html

## GR-1: Mahogany Rich QEMscan image 10µm res.



- Dominantly interlaminated dolomite and illite
- Background assumed to be mostly organic matter
- Note laminated nature of organic matter





## GR-2: Mahogany Lean QEMscan image 10µm res.



- Dominantly calcite, dolomite, and micrite (carbonate mud)
- Suprisingly little background, very little organic matter



## GR-2 BSE image 10µm res.



## GR-3: Upper R6 rich QEMscan image 10µm res.



- Dominantly interlaminated and interbedded dolomite and illite
- Significant organic matter content concentrated in organic rich laminations



## GR-3 BSE image 10µm res.



## GR-4: Lower R8 rich QEMscan image 10µm res.

Mineral Name	
Calcite	43.42
Illite/Muscovite	25.11
Dolomite	18.85
Quartz 📃	6.70
Plagioclase	3.12
Background	1.34
Pyrite	0.87
K_Feldspar	0.83
Other Metal (S) Phases	0.78
Trap Definitions	0.29
Apatite	0.02
Others	0.01

- Interlaminated calcite/ dolomite and illite
- Low organic matter (background) content



## GR-4: Lower R8 rich BSE image 10µm res.



### GR-5: R5 rích QEMscan image 10µm res.

#### **Mineral** Name

Illite/Muscovite	40.60
Dolomite	16.07
Plagioclase	14.42
🔲 Quartz	13.48
Calcite	7.65
K_Feldspar	4.28
Other Metal (S) Phases	3.14
Trap Definitions	0.17
Pyrite	0.16
🔜 Background	0.08
Others	0.02
Apatite	0.01

- Interlaminated dolomite and illite
- Low organic matter (background) content



## GR-5: R5 rich BSE image 10µm res.



# Conclusions

- 1. QEMscan analysis reveals mineralogic textures dominated by dolomite, illite, and calcite.
- 2. A few interpretations are made in regards to the documented compositional results generated automatically by the QEMscan:
  - "Background" is assumed to reflect organic matter content, as organic carbon is below the instrument detection limit.
  - "Plagioclase" is interpreted as an iron-rich variant of illite, and not plagioclase.
  - o "Quartz" content is likely biogenic silica rather than detrital quartz.
- 3. Variations in mineralogy between samples documented here are broadly in line with stratigraphic variations as predicted from detailed geologic description (Birgenheier & Vanden Berg, 2011).
- 4. The nature of intersample variability needs to be further evaluated with additional samples from the same intervals.

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