

# Oil & Natural Gas Technology

DOE Award No.: DE-FE0001243

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

### Quarterly Progress Report (July – September 2013)

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

November 6, 2013



Office of Fossil Energy

Acknowledgment: "This material is based upon work supported by the Department of Energy under Award Number DE-FE0001243."

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## EXECUTIVE SUMMARY

The Clean and Secure Energy from Domestic Oil Shale and Oil Sands Resources program, part of the research agenda of the Institute for Clean and Secure Energy (ICSE) at the University of Utah, is focused on engineering, scientific, and legal research surrounding the development of these resources in Utah.

In Task 2, which focuses on outreach and education, the entire ICSE collection of documents related to oil shale and oil sands (the “repository”) was made available in the University of Utah Marriott Library USpace collection. Other outreach efforts include conference presentations and journal publications by various ICSE researchers; see the “RECENT AND UPCOMING PRESENTATIONS/PUBLICATIONS” section of this document.

Task 3 focuses on utilization of oil shale and oil sands resources with CO<sub>2</sub> management. Subtask 3.1 researchers submitted a paper entitled “Oxyfiring with CO<sub>2</sub> capture to meet low-carbon fuel standards for unconventional fuels from Utah” to the International Journal of Greenhouse Gas Control. The Subtask 3.2 research team is developing a two-step process for modeling an oxy-fired furnace fired by a burner with complex geometry. The burner geometry has been fully resolved using the commercial software STAR-CCM+. Subtask 3.3 and 3.4 researchers are developing a model for conventional oil and gas development in the Uinta Basin based on prior drilling activity and energy (oil and gas) prices. This model will be added to a system dynamics model that computes regional impacts of conventional and unconventional fuel development, including CO<sub>2</sub> emissions.

Task 4 projects are related to liquid fuel production by in-situ thermal processing of oil shale. Subtask 4.1, 4.2, and 4.8 researchers continued work on drafting final reports. The Subtask 4.3 and 4.9 research teams are preparing two manuscripts related to various analyses of the Skyline 16 core for publication in Energy & Fuels. Additional work comparing rates of kerogen pyrolysis at different heating rates reported by Dr. Fletcher’s group and Dr. Deo’s group was performed and significant differences were found at the low heating rates (1 K/min). Sources for this discrepancy will be investigated. Subtask 4.7 researchers studying the geomechanical reservoir state completed triaxial and creep testing on several Skyline 16 core samples and will continue the testing required to complete their experimental matrix.

Task 5 projects provide analyses of the environmental, legal, economic, and policy framework. Researchers are nearing completion of a draft report for the one remaining subtask, an analysis of policy and economic issues associated with using simulation to assess environmental impacts.

All Task 6 projects (economic and policy assessment of a domestic unconventional fuels industry) are now complete. The Subtask 6.1 models and data are available for download at <http://www.oilshalesands.utah.edu/leftnavid3page28>. The Subtask 6.2 policy analysis of the Canadian oil sands experience was revised in accordance with comments received from Robert Vagnetti and then submitted.

Task 7 researchers are focused on research relevant to their industrial partner, American Shale Oil (AMSO). The Subtask 7.1 team continued with segmented linearization and development of constitutive modeling surfaces on AMSO data, initiated development of a stress-strain-temperature-grade-confining pressure response surface, and began subsidence assessments using the response surface data. The Subtask 7.3 research team conducted refluxing simulations inside the lower lateral of the AMSO heater test. They were able to qualitatively demonstrate that temperatures measured at the heater wall are substantially greater than temperatures at the shale boundary surrounding the AMSO pilot test formation interval.

## PROGRESS, RESULTS, AND DISCUSSION

### Task 1.0 - Project Management and Planning

There were no schedule/cost variances or other situations requiring updating/amending of the Project Management Plan (PMP) in this quarter. Internal budgeting reallocation occurred during this quarter as described under Tasks 3.2 and 4.3.

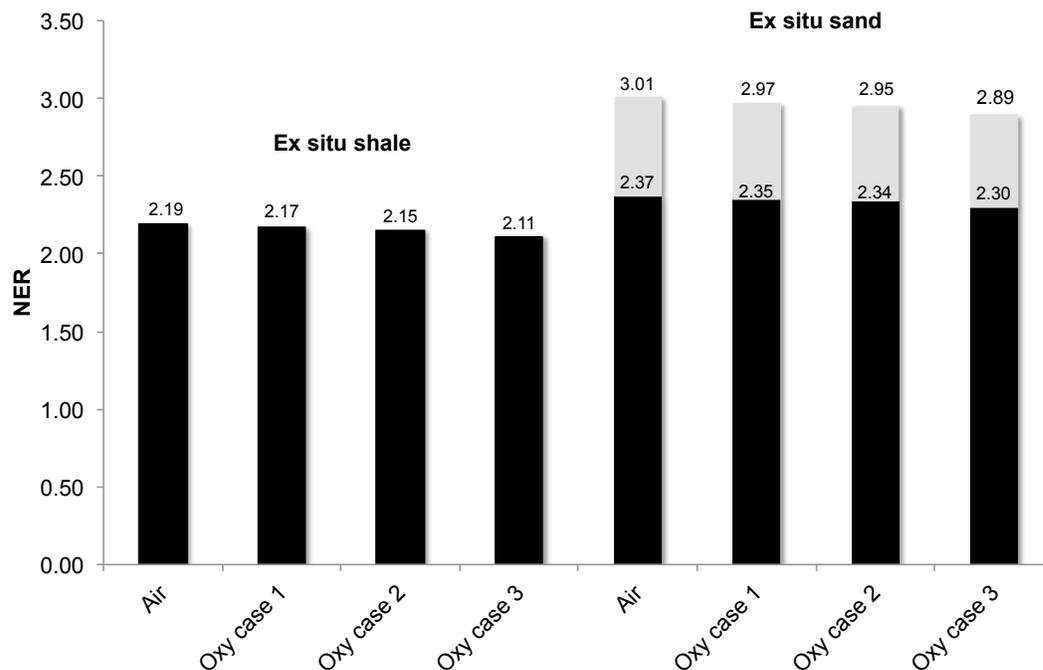
### Task 2.0 -Technology Transfer and Outreach

Task 2.0 focuses on outreach and education. Efforts this quarter focused on completion and verification of the transfer of the ICSE DSpace collection to the Marriott Library ICSE USpace collection. All of the ICSE DSpace items are now accessible through USpace, and ICSE items gathered since the transfer was initiated have been uploaded to the USpace collection.

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

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

During this quarter, the team completed the final Phase I deliverable by submitting a paper to the International Journal of Greenhouse Gas Control. This paper describes the use of oxy-firing to meet a low-carbon fuel standard for transportation fuels produced from Utah unconventional fuels (oil shale or “shale” and oil sands or “sand”). During the final refinement of the results, the team identified and resolved an inconsistency with the hydrotreater energy requirements. Many of the highlights were discussed in the previous quarterly report. Figure 1 illustrates the updates to net energy return (NER) and net external energy returns (NEER) for several oxy-firing cases.



**Figure 1.** Point-of-consumption NER and NEER estimates for the air-fired baseline and three oxy-fired cases. For the shale cases, NER and NEER are equal, but for the sands cases NER

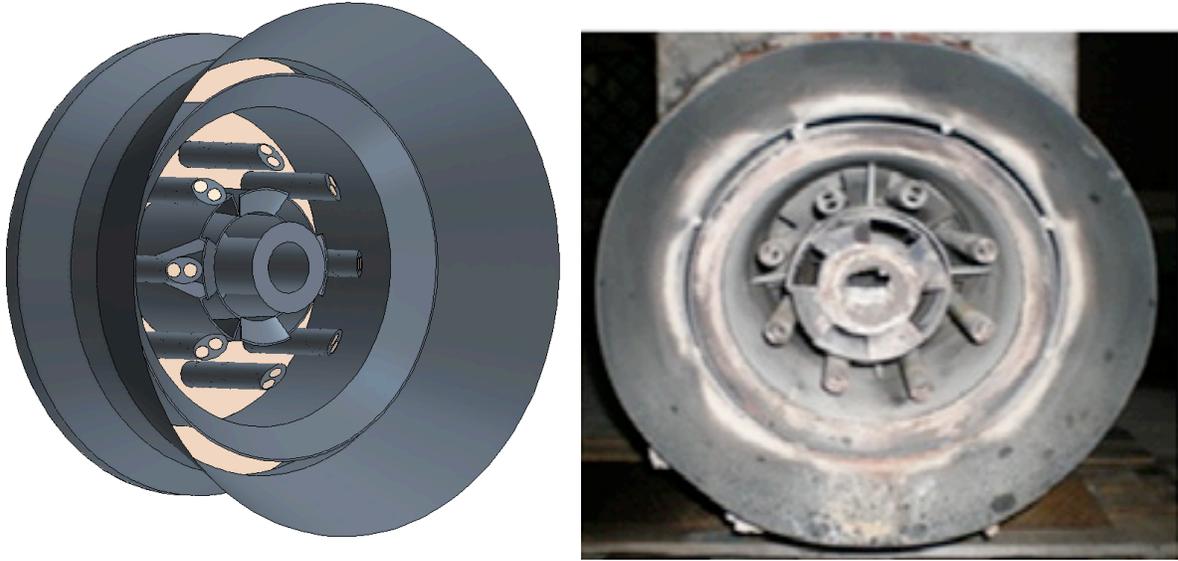
(lower value) and NEER (higher value) are both presented. In situ sand is excluded because the baseline NER is less than 1.

The NERs for gasoline produced from the ex situ sands and shale, the baseline (air-fired) and oxy-fired cases are lower than the US-average, point-of-consumption energy return on invested (EROI) of 6–10 (Cleveland, 2005). The NERs for these unconventional resources will likely be a significant barrier to their commercial production. The range of NERs in this study is generally consistent with other studies of unconventional fuels. Cleveland also reports an NER for refined fuel produced from in situ and ex situ production of oil shale of approximately 1.5. They also summarize EROIs at the point of consumption calculated for oil shale processes and report EROIs ranging from 1.2–7 for in situ shale and 1.1 to greater than 10 for ex situ shale. A direct comparison with some of these studies is difficult because system boundaries differ. Brandt (2008, 2009) is the most widely cited source regarding NERs and GHG emissions for oil sands and shale. He reports NERs ranging from 1.2–1.6 for in situ oil production of refined fuel from oil shale. Although the estimated NER for gasoline produced by in situ processing of shale in this study is lower than those reported by Brandt (2008), shale richness and permeability are critical factors in both the energy required and the associated GHG emissions from this scenario. Brandt (2009) also reports an NER for the ATP process (ex situ shale) of 1.1–1.8, and this study's baseline NER for ex situ shale of 2.19 is slightly higher. However, the NER is consistent with this study's lower GHG emissions, which are on the low end of those reported by Brandt. The baseline NER of 2.37 for gasoline produced from ex situ oil sand is close to the NER reported by Brandt et al. (2013) of 2.81 for point of consumption product produced from Canadian oil sands. Inman et al. (2013) report an EROI of 1.6 for Canadian oil sands.

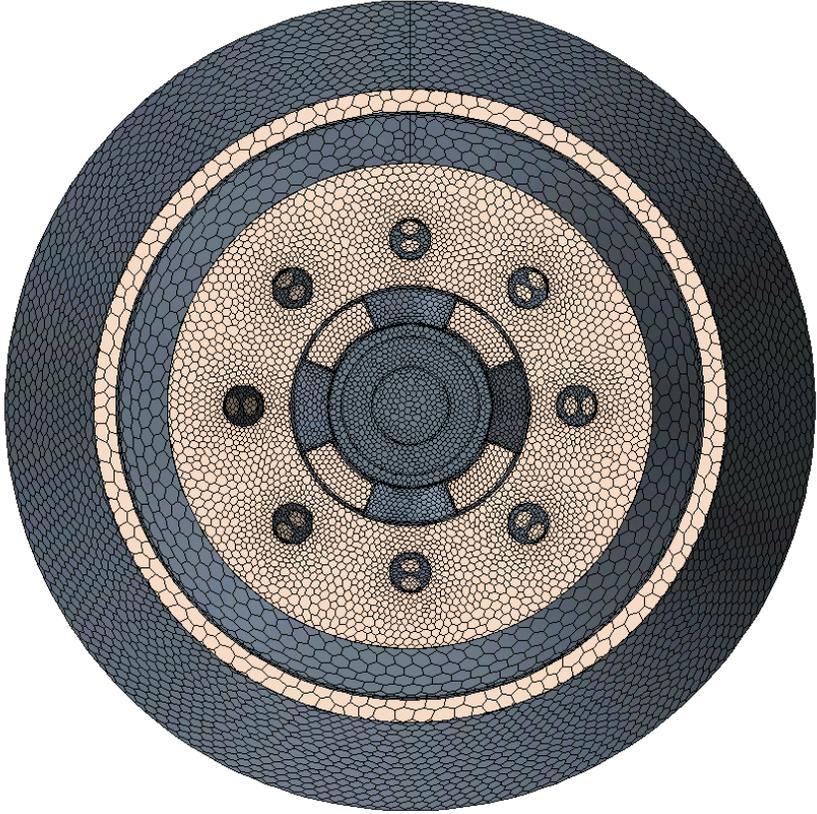
Studies on the effect of oxyfiring with CO<sub>2</sub> capture on NER are limited. However, Corsten et al. (2013) recently summarized the effect of carbon capture and storage from several life-cycle assessments studies and report a 16–44% reduction in NER associated with the addition of CO<sub>2</sub> capture for coal-fired power plants and a lower reduction in NER for natural gas power plants for CO<sub>2</sub> capture of 88–95% of the CO<sub>2</sub>. This study shows a reduction in NER of 1–4% associated with a 7–34% reduction in WTW GHG emissions. It is also worth noting that adding carbon capture to reduce GHG emissions increases other environmental impacts due to increased energy demand and fuel consumption (Zapp et al., 2012).

### Subtask 3.2 - Flameless Oxy-gas Process Heaters for Efficient CO<sub>2</sub> Capture (PI: Jennifer Spinti)

During the time period that this project has been on hiatus, a bug was discovered in the simulation tool that affected cases with complex geometries. The TEA-C burner used to fire the FOSPER furnace in the oxy-gas experiments being studied has a very complex geometry that required the specification of multiple overlapping geometry objects on the boundary of the computational mesh. Because of the bug, the mass flow rates through these areas of overlapping geometry may have been incorrect in previous ARCHES simulations. For this reason, a new, loosely-coupled approach is required to complete this project. In this approach, the elements of the burner geometry are fully resolved in the commercially-available code STAR-CCM+ and the flows of natural gas and of recycled flue gas spiked with oxygen through these elements are computed. The temporally-filtered output from this simulation is then spatially filtered to match the mesh resolution of the ARCHES computational mesh. Finally, the filtered output is used as the inlet condition for the ARCHES simulation. Figures 2 and 3 show the STAR-CCM+ computational mesh that has been developed for the TEA-C burner.



**Figure 2.** (left) Computational domain developed for the TEA-C burner in STAR-CCM+. (right) Photograph showing actual TEA-C burner.



**Figure 3.** STAR-CCM+ computational mesh (plan view) used for simulations of fluid flow through the TEA-C burner.

The due date of the final deliverable for this project has been extended to August of 2014 and money has been rebudgeted from Subtask 7.2 (terminated) to pay for the additional work required to produce the handoff files and to perform the matrix of simulations needed for the validation/uncertainty quantification analysis.

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

Based on the literature review of constraints in the Uinta Basin to oil and gas production completed during the second quarter of 2013, the project team has decided to shift the model of oil and gas development in the Basin from a constrained model to an empirical model. The goal of the constrained model was to develop an exhaustive list of potential constraints to development (economics/profitability, drill rig counts, permitting, water availability, etc.) and to predict drilling activity based on those constraints. This model proved unusable for several reasons. First, after completing a review of the all the potential constraints, no “hard” constraints were found. That is, all of the constraints could change over time in response to demands for additional oil production. Second, the “soft” upper limit on all of the constraints was too high to impact production growth in the Basin. The model assumed that the amount of drilling that occurred in any time step would be equal to the capacity of the set of constraints at that point in time. As a result, in the first time step where drilling a well was predicted to be profitable (the economic constraint), the model predicted a huge number of wells would be drilled. Several methods for slowing production growth were discussed, but none were found to be suitable. Finally, after reviewing other methods for modeling oil and gas development (Walls, 1992; M. Managi and Opaluch, 2004; Lynch, 2003; Kemp and Kasim, 2003; Kaiser et al., 2004, Huntington et al., 2013, , Eckbo et al., 1977) team members concluded that none of the constrained or mechanistic models in the literature were any more successful at predicting development than empirical models.

As a result, the project team has decided to switch to an empirical model of oil and gas development in the Uinta Basin that predicts the number of wells drilled based on prior drilling activity and energy (oil and gas) prices. This type of model is based on the method used by Moroney (1997) and proposes the following type of empirical relationship between energy prices and past and present drilling activity:

$$W_t = a + b \cdot W_{t-1} + c \cdot P_t \quad (1)$$

where  $W_t$  is the number of wells drilled in time step  $t$ ,  $W_{t-1}$  is the number of wells drilled in the previous timestep,  $P_t$  is the price of the fluid produced by the well (either oil or gas), and  $a$ ,  $b$ , and  $c$  are empirically-fitted coefficients. Using the extensive amount of data available from the State of Utah’s Division of Oil, Gas and Mining (DOGGM), team members are working to fit Equation (1) to each of the oil and gas fields in the Uinta Basin based on historical data from the 1999 – 2013 time period. By disaggregating the fit of Equation (1) to each field, the project team aims to adequately encompass all the factors and constraints unique to each field in the Basin. Production volumes will similarly be fitted to each field (for both oil and gas) using a hyperbolic decline curve of the form:

$$q(t) = q_o (1 + d \cdot e \cdot t)^{-\frac{1}{d}} \quad (2)$$

where  $q$  is the fluid (oil or gas) production rate at time  $t$ ,  $q_o$  is the initial production rate, and  $d$  and  $e$  are fitted coefficients. This empirical model comprising the fitting of Equations (1) and (2) to all fields in the Basin for both oil and gas wells will be used to estimate future oil and gas development in the Uinta Basin based on forecasted oil and gas prices from the Energy Information Administration. By the end of this quarter, team members had successfully imported

into the statistical software package R all of the input data to the model from the DOGM database. They are currently working on the regression analysis of the datasets for each field.

#### Subtask 3.4 - V/UQ Analysis of Basin Scale CLEAR<sub>uff</sub> Assessment Tool (PI: Jennifer Spinti)

The Subtask 3.3 includes a summary of all activities associated with Subtasks 3.3 and 3.4.

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

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

In the past quarter, researchers have continued to run simulations representing the rubblized section of the oil shale formation. However, the majority of their effort during this quarter went to completing tasks associated with Subtask 7.3, which were presented at the 33<sup>rd</sup> Oil Shale Symposium in Golden, Colorado, held on October 14-16, 2013. The research team has now refocused its efforts on this subtask and will be completing the final report by the deliverable due date (December 31, 2013).

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

The research team has asked for an extension on the final project deliverable to March 31, 2014. A draft will be completed by the end of November, and the extension will be used to review and revise the draft.

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

There are two deliverables left for this project: (1) A Topical Report describing CPD/shale & oil generation (pyrolysis) models including summary of their applications/limitations (due August 2013) and (2) a paper on combined kerogen/bitumen structures & CPD reaction model submitted to a journal such as Energy & Fuel (joint deliverable with Subtask 4.9, due August 2013).

This subtask received additional funds from Subtask 7.2, which was terminated. The project team requests that the due date for the first deliverable, a Topical Report describing CPD/shale and oil generation models including a summary of their applications/limitations, be extended to September 30, 2014. With the increased budget and the extension for the deliverable, the following additional work will be completed:

- Seek additional literature data and perform further experiments to resolve the differences between the Fletcher group Thermogravimetric Analyzer (TGA) data and the Deo group TGA data at 1 K/min. Currently the temperature at which the reactions take place at 1 K/min differ by 50° to 100°C. Calibration using Curie point metals and a magnet will be an important part of these experiments.
- Perform some experiments at lower heating rates.
- Extend the Chemical Percolation Devolatilization (CPD) model for oil shale to include additional chemistry specific to oil shale. Alan Burnham of American Shale Oil (AMSO) has expressed interest in working with Prof. Fletcher and Prof. Pugmire on this project.

Researchers spent this past quarter working on two papers that will fulfill the second deliverable:

1. A paper on the nuclear magnetic resonance (NMR) analyses of the three oil shale samples studied by the group (GR1-3), as well as the bitumen extracted and the demineralized kerogen. This paper was submitted to *Energy and Fuels* and the review comments have been received. Team members are currently working on a response to the review comments, including the citation of more papers by one of the reviewers.
2. A paper on the analysis of the pyrolysis products from kerogen, including NMR analyses of the char and tar samples obtained at different temperatures, gas chromatography/mass spectrometry analyses of the tar samples, and Fourier transform infrared analysis of the light gases. This paper is 90% completed and will be submitted as Part 2 of the first paper sent to *Energy and Fuels*.

In other work, Prof. Pugmire, recently returned from his missionary service in Africa, together with Prof. Fletcher at Brigham Young University, has been assembling data from various ICSE investigators. Based on Prof. Pugmire's recommendation, a draft paper of previous data on Colorado oil shale pyrolysis was completed and submitted to the journal *Industrial and Engineering Chemistry Research*. This paper was reviewed, following which significant changes were made. The revised paper was accepted and is now available online as an "ASAP" article before appearing in the journal (Hillier *et al.*, 2013). Finally, Prof. Fletcher presented this work at the 33<sup>rd</sup> Oil Shale Symposium in Golden, Colorado. The presentation abstract is included in Appendix A.

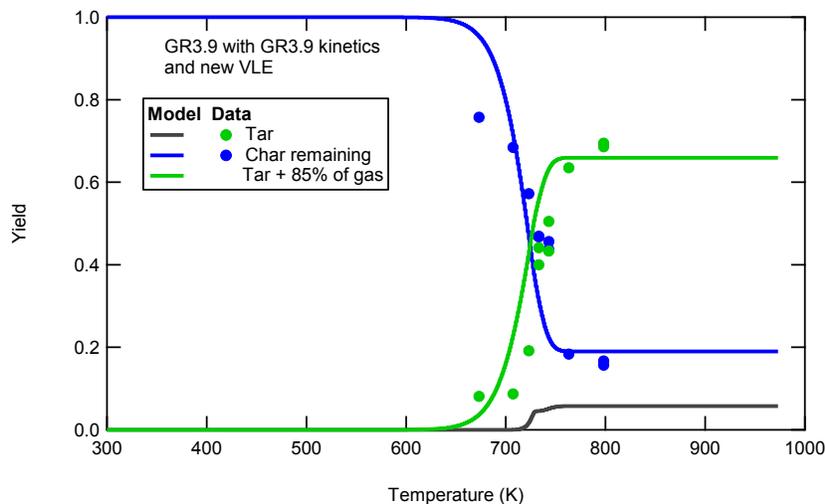
#### *Comparison of Oil Shale Pyrolysis Models*

A comparison of the rates of pyrolysis at different heating rates reported by Dr. Fletcher's group and Dr. Deo's group was performed last quarter, and significant differences were found at the low heating rates (1 K/min). Sources for this discrepancy have not yet been found yet but will be the topic of research during the coming quarter.

#### *CPD Model*

Last quarter a simple vapor pressure correlation was developed for the CPD model to describe the *n*-alkanes being released. Additional CPD runs were made for a presentation at the 33<sup>rd</sup> Oil Shale Symposium in Golden, Colorado. It was found that the rate parameters from the TGA experiments could be applied in the CPD model along with the measured lattice parameters derived from NMR analyses of the demineralized kerogen.

CPD predictions of yields from kerogen pyrolysis are shown in Figure 4 together with experimental data collected in the kerogen retort (discussed in previous quarterly reports). The current version of the CPD model does not permit detached side chains to formally be part of the condensable tar (gray line in Figure 4). However, since side chains in kerogen are 12-15 aliphatic carbons in length, these long chains condense and are part of the tar (or oil). The assumption that 85% of the side chains condense gave good agreement in the tar yield for the GR3.9 sample (green line in Figure 4) as well as good agreement with data for the GR1.9 and GR2.9 samples (not shown here). Team members had good discussions with Alan Burnham and others at the Oil Shale Symposium about interest in this chemical structure-based approach to modeling oil shale pyrolysis.



**Figure 4.** CPD predictions of kerogen pyrolysis for the GR3.9 sample at 10 K/min compared with data from the kerogen retort taken at 10 K/min.

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)

This project has been completed.

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

This project has been completed.

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

This project has two outstanding milestones: (1) complete experimental matrix and (2) complete thermophysical and geomechanical property data analysis and validation. Based on progress made to date, the research team has asked for an extension on both milestones. The new completion date for the completion of the experimental matrix is March 31, 2014 and for the data analysis and validation is April 30, 2014.

*Experimental Matrix*

Background testing and shakedown of the apparatus was performed on White River oil shale samples and reported previously. The Skyline 16 oil shale samples have been prepared and computed tomography (CT) scans have been taken. The tests that have been completed thus far are summarized in Table 1.

**Table 1.** Completed tests on Skyline 16 oil shale samples that are useful for analyses and interpretation.

Sample ID	Depth (ft)	Orientation	Testing	Confining Pressure (psi)	Temperature (°F)
SL16-462-H <sup>1</sup>	462	Horizontal	Triaxial		
SL16-486-H	486	Horizontal	Triaxial	1000	750
SL16-549-H	549	Horizontal	Creep	950	750
SL16-462-V	462	Vertical	Triaxial	500	750
SL26-486-V	486	Vertical	Triaxial	1000	750
SL16-549-V	549	Vertical	Triaxial	800	250
WR6		Horizontal	Creep	550	750

#### 1. Issues with LVDTs

Additional Skyline samples have been requested to continue triaxial testing. The project team will be doing some minor equipment modifications as well as unconfined compression and creep tests at temperature. Creep testing may be more realistic of formation response during slow heating.

#### *Thermophysical and Geomechanical Property Data Analysis and Validation*

Several elements of this milestone have been completed, including the literature compilation and evaluation. The database has also been constructed and will be fully populated once testing is finished.

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

In this quarter, the finalized individual core logs along with associated geochemical data were still being updated in preparation for upload to the ICSE data repository. In addition, Michael Vanden Berg at Utah Geological Survey began writing the Topical Report on the geologic model that has been developed. An extension of the completion date for these deliverables to December 31, 2013 is requested.

#### Subtask 4.9 - Experimental Characterization of Oil Shales and Kerogens (PI: Julio Facelli)

The final deliverable, a series of two papers on the combined kerogen/bitumen structures and the CPD reaction model, is nearing completion. Updates on this joint deliverable with Subtask 4.3 are found in that subtask's summary. Additionally, Prof. Pugmire presented work from this subtask at the 33<sup>rd</sup> Oil Shale Symposium in Golden, Colorado. An abstract for his presentation is included in Appendix A.

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

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

This project has been completed.

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

This project has been completed.

Subtask 5.3 - Policy and Economic Issues Associated with Using Simulation to Assess Environmental Impacts (PI: Robert Keiter, Kirsten Uchitel)

Efforts this quarter focused on drafting of the topical report. A draft version of the topical report will be sent to Robert Vagnetti by November 15, 2013.

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

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

The milestone to upload all process models used and data collected to the ICSE website was completed on August 15, 2013. A compressed file containing both the model spreadsheet and instructions on its setup and use is available for download at <http://www.oilshalesands.utah.edu/leftnavid3page28>. This project is now finished.

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

The topical report was edited in accordance with comments received from Robert Vagnetti at NETL and was submitted in final form to OSTI. The project is now completed.

Subtask 6.3 – Market Assessment Report (PI: Jennifer Spinti)

This project has been completed. In addition to the \$80K approved for re-budget to Subtask 6.3 in the no-cost extension, an additional \$17K was required to complete the assessment. The funding was available in the Management - Task 1 due to the severance of three computing-based positions. This brings the total federal cost of the assessment to \$399,488.

Jon Wilkey presented this work at the 33<sup>rd</sup> Oil Shale Symposium in Golden, Colorado. The abstract for the presentation is included in Appendix A.

## **7.0 – Strategic Alliance Reserve**

Subtask 7.1 – Geomechanical Model (PI: John McLennan)

The milestone to make experimental recommendations has been completed. As the project team proceeded through testing development in Subtask 4.7, the following recommendations were developed for Subtask 7.1:

- A few triaxial compression tests need to be run to help fill in the matrix for the response curves.
- The triaxial tests at high temperature should be completed first.
- Because of the low thermal conductivity, dramatic in-situ changes (e.g. mechanical deformation) will have happened to the formation long before pyrolysis temperatures are reached. This situation mandates running more low temperature tests.
- Realistic boundary conditions will be more like creep testing than triaxial compression. In creep testing, the samples are loaded to initial in-situ stress conditions. They will be stable under these conditions. Then the temperature is increased to simulate the action of the heaters. The failure behavior of the sample is monitored to see when and at what temperature catastrophic deformation of the sample occurs.
- Evaluation using unconfined compression will be continued. Additionally, the influence of the absolute temperature and the rate of heating will be studied.

An extension of the completion dates for all remaining project milestones and deliverables is requested as listed below.

- (milestone) Infer permeability-porosity-temperature relationships, develop model that can be used by other subtasks - January 2014
- (milestone) Basic reservoir simulations to account for thermal front propagation - August 2014
- (milestone) Evaluation of flow mechanics - August 2014
- (deliverable) Version 1 of geomechanical model with report - September 2014

To complete the milestone to infer permeability-porosity-temperature relationships and develop a model, researchers have added triaxial testing (on an AMSO sample, CT scanned last quarter along with the Skyline samples) from the work being done for Subtask 4.7 to increase the mechanical properties data available. The testing in Subtask 4.7 will also provide some basis for inferring permeability and porosity relationships with temperature.

Segmented linearization and development of constitutive modeling surfaces is proceeding. The data that has been generated at the University of Utah is being amalgamated with the AMSO data to develop a stress-strain-temperature-grade-confining pressure response surface. From this response surface, stress-strain plots can be inferred based on independent parameters including temperature, confining pressure and grade. A Ph.D. student, Thang Tran, is working on this part of the project with an undergraduate researcher.

The milestone to perform basic reservoir simulations will most likely employ commercial software from Itasca and CMG. Some complimentary testing is planned with reservoir models developed at the University of Utah (ARTS).

Subsidence and compaction are being evaluated to meet the upcoming deliverable, "Version 1" of the geomechanical model. An MS candidate, Walter Glauser, is initiating work on subsidence assessments using the response surface data that has been generated.

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

Project has been terminated.

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

The milestone to perform a Generation 2 simulation that incorporates kinetic compositional models has been delayed until January 2014 as AMSO engineers have been more interested in simulation work that supported their efforts in heater design. Based on past results of the heat dissipation simulation through the formation, the research team decided to create a simulation of the refluxing in the lower lateral to better predict the input boundary condition for the heat dissipation simulations.

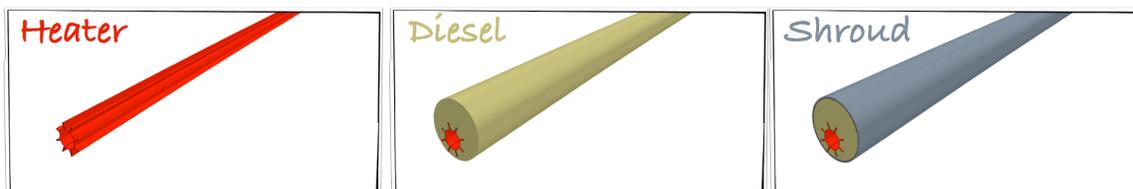
Previous results from the heat dissipation simulation indicated that experimental temperatures, measured by AMSO at their tomography wells, were over-predicted throughout the formation. Therefore, after discussion with AMSO engineers, researchers created a detailed simulation of the heater in the lower lateral well, the liquid surrounding the heater, and the steel shroud. The shroud protects the heater from formation subsidence during heater tests and subsequent retorting.

The experimental heater chosen for the simulation is shown in Figure 5. It is important to note that, the heater design shown in Figure 5 was only used for small tests and not for the actual heater test at the AMSO site. However, while the heater geometry in the simulation is not an exact match of the actual heater, physical processes occurring inside the lower lateral are conceptually equivalent to the actual heater test. Therefore, the simulation results, while not quantitative, can be used to draw qualitative conclusions.



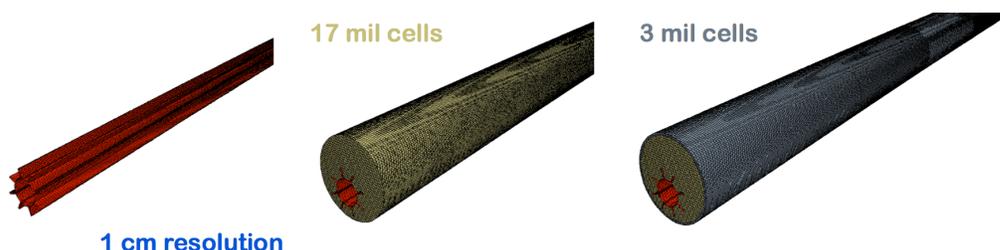
**Figure 5.** Heater used small experimental tests at the AMSO site.

The computer-aided design (CAD) representation of the heater, as well as the surrounding diesel and shroud, are shown in Figure 6. The thermocouple, which is attached to the heater wall, measures the temperature of the heater, not the temperature at the formation boundary. Therefore, the outside shroud temperature in the simulation can be used to estimate the amount of heat which goes into the formation at specific locations along the lower lateral well.



**Figure 6.** CAD representation of the experimental heater in the simulations, along with the diesel and shroud, all inside the lower lateral well.

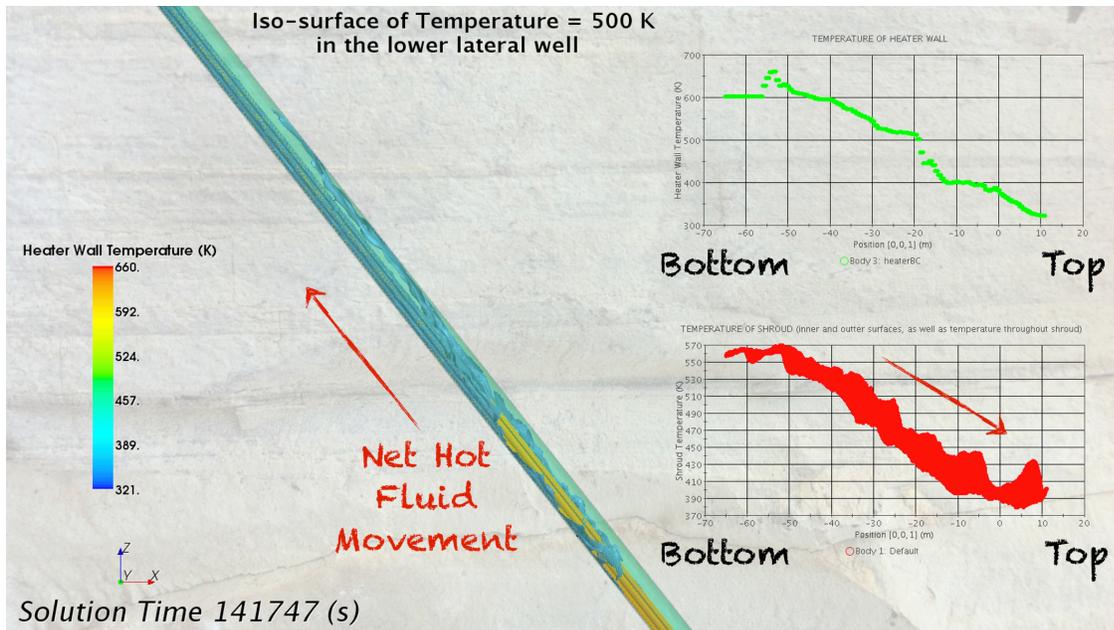
The computational mesh to resolve the heater, diesel, and the shroud is shown in Figure 7. The mesh resolution is 1 cm, which translates into 17 million cells to resolve the diesel fuel and 3 million cells to resolve the steel shroud. The computational mesh captures the entire length of the lower lateral well, from the bottom of the well to the packer which seals the heater test region from the aquifer located above the AMSO test section. Therefore, the simulation resolves a length of approximately 100 m at a resolution of 1 cm. Because of the very fine resolution required to capture the unsteady fluid movement, the simulation ran on 600 processes for two weeks to simulate the three months of heating by AMSO. The LES WALE model was used to capture the unsteady convective fluid time scales with time steps of 10 seconds.



**Figure 7.** Computational mesh used to resolve the heater, diesel, and shroud.

Simulation results of the iso-contours of 500 K temperatures inside the diesel are shown in Figure 8. The figure also shows plots of the temperature at the heater wall (green line in the upper right plot) and of the temperature on both the inside and outside surfaces of the shroud (red line in the bottom right plot). As can be seen from Figure 8, the outside shroud temperature lags behind the heater temperature by about 50 to 100 K. Furthermore, the peak in heater temperature (green line) at a position of about -55 m is clearly missing from the temperature at the shroud surface (red line). This result means that temperatures measured at the heater are redistributed in the diesel, which acts as a heat transfer buffer. Hence, the heat that is measured by the thermocouple attached to the heater greatly over-predicts temperatures and therefore the amount of heat that actually goes into the formation. These results at least partly explain why previous heat dissipation simulations over-predicted the temperatures at the tomography wells when compared to experimental measurements.

This work was presented at the 33<sup>rd</sup> Oil Shale Symposium in Golden, Colorado. The presentation abstract is included in Appendix A.



**Figure 8.** Refluxing simulations of diesel heated by heater inside the lower lateral well.

## CONCLUSIONS

Research performed under the various subtasks has been presented at several recent conferences, including the American Association of Petroleum Geologists Annual Meeting and the 33<sup>rd</sup> Oil Shale Symposium. In addition, several papers were either submitted for publication or published during the quarter in journals such as *Industrial and Engineering Chemistry Research*, *International Journal of Greenhouse Gas Control*, and *Energy & Fuel*. Project timelines were extended on Subtasks 3.2, 4.2, 4.3, 4.7, 4.8, 4.9, 7.1, and 7.3 to better match the stage of each project. Subtasks 4.1, 4.8, 4.9, and 5.3 will be completed in the next quarter.

# COST PLAN/STATUS

Baseline Reporting Quarter - PHASE I	Yr. 1								Yr. 2			
	Q1		Q2		Q3		Q4		Q5		Q6	
	7/1/09 - 12/31/09		1/1/10 - 3/31/10		4/1/10 - 6/30/10		7/1/10 - 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
<b>Baseline Cost Plan</b>												
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
<b>Actual Incurred Cost</b>												
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
<b>Variance</b>												
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.

Baseline Reporting Quarter - PHASE II	Yr. 2				Yr. 3							
	Q7		Q8		Q9		Q10		Q11		Q12	
	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
<b>Baseline Cost Plan</b>												
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
<b>Actual Incurred Cost</b>												
Federal Share	449,459	3,078,729	314,813	3,393,542	271,897	3,665,439	267,784	3,933,223	191,438	4,124,661	232,367	4,357,028
Non-Federal Share	48,902	699,537	48,835	748,372	105,695	854,067	40,652	894,719	33,092	927,811	44,294	972,105
Total Incurred Costs	498,361	3,778,266	363,648	4,141,914	377,592	4,519,506	308,436	4,827,942	224,530	5,052,472	276,661	5,329,133
<b>Variance</b>												
Federal Share	262,926	694,297	312,610	1,006,907	-124,446	882,461	-120,333	762,128	-43,987	718,141	13,080	731,221
Non-Federal Share	129,198	243,972	108,019	351,991	-68,832	283,159	-3,789	279,370	3,771	283,141	14,612	297,753
Total Variance	392,124	938,269	420,629	1,358,898	-193,278	1,165,620	-124,122	1,041,498	-40,216	1,001,282	27,692	1,028,974

Baseline Reporting Quarter - PHASE II	Yr. 4								Yr. 5			
	Q13		Q14		Q15		Q16 - REVISED		Q17		Q18	
	10/01/12 - 12/31/12		01/01/13 - 03/31/13		04/01/13 - 06/30/13		07/01/13 - 09/30/13		10/01/13 - 12/31/13		01/01/14 - 03/31/14	
	Q13	Total	Q14	Total	Q15	Total	Q16	Total	Total	Total	Total	Total
<b>Baseline Cost Plan</b>												
Federal Share	146,824	5,235,073	146,824	5,381,897	146,824	5,528,721	-471,238	5,057,483		5,214,733		5,371,983
Non-Federal Share	36,705	1,306,563	36,705	1,343,268	36,705	1,379,973	-211,982	1,167,991		1,221,475		1,274,959
Total Planned	183,529	6,541,636	183,529	6,725,165	183,529	6,908,694	-683,220	6,225,474		6,436,208		6,646,942
<b>Actual Incurred Cost</b>												
Federal Share	128,349	4,485,377	180,613	4,665,990	233,732	4,899,722	157,761	5,057,483		5,057,483		5,057,483
Non-Federal Share	79,871	1,051,976	62,354	1,114,330	51,708	1,166,038	1,953	1,167,991		1,167,991		1,167,991
Total Incurred Costs	208,220	5,537,353	242,967	5,780,320	285,440	6,065,760	159,714	6,225,474		6,225,474		6,225,474
<b>Variance</b>												
Federal Share	18,475	749,696	-33,789	715,907	-86,908	628,999	-628,999	0				
Non-Federal Share	-43,166	254,587	-25,649	228,938	-15,003	213,935	-213,935	0				
Total Variance	-24,691	1,004,283	-59,438	944,845	-101,911	842,934	-842,934	0				

Note: Baseline Cost Plan adjusted in Q16 to reflect NCE projections.

Baseline Reporting Quarter - PHASE II	Yr. 5			
	Q19		Q20	
	04/01/14 - 06/30/14		07/01/14 - 09/30/14	
	Q19	Total	Q20	Total
<b>Baseline Cost Plan</b>				
Federal Share		5,529,233		5,662,515
Non-Federal Share		1,328,443		1,415,879
Total Planned	0	6,857,676	0	7,078,394
<b>Actual Incurred Cost</b>				
Federal Share		5,057,483		5,057,483
Non-Federal Share		1,167,991		1,167,991
Total Incurred Costs	0	6,225,474	0	6,225,474
<b>Variance</b>				
Federal Share	0	471,750	0	605,032
Non-Federal Share	0	160,452	0	247,888
Total Variance	0	632,202	0	852,920

## 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-13	N/A	Decision has been made to disband EAB
	Hold final project review meeting	Jun-13		NCE will delay this meeting until 2014
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	Mar-14		Milestone date has been changed to reflect new project timelines
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	Sep-12	Oct-12	Report attached as appendix to Oct. 2012 quarterly report
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 of V/UQ methodology for conventional oil development in Uinta Basin	Nov-13		Due date has been revised to reflect personnel availability
	Demonstrate full functionality for conventional & unconventional oil development in Uinta Basin	Mar-14		
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			

<b>ID</b>	<b>Title/Description</b>	<b>Planned Completion Date</b>	<b>Actual Completion Date</b>	<b>Milestone Status</b>
	Expand modeling to include reaction chemistry & study product yield as a function of operating conditions	Feb-12	Mar-12	Discussed in April 2012 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	Discussed in Jan. & July 2012 quarterly reports
	Complete examination of pore-level change models & their impact on production processes in both commercial & new reactive transport models	Jun-12	Jun-12	Discussed in July 2012 quarterly report
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	Sep-12	Discussed in Oct. 2012 quarterly report
	Collection & chemical analysis of condensable pyrolysis products from demineralized kerogen	May-12	Sep-12	Discussed in Oct. 2012 quarterly report
	Complete model to account for heat & mass transfer effects in predicting product yields & compositions	Jun-12	Jun-12	Discussed in July 2012 quarterly report
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 April 2012 quarterly report for 1 loading condition; samples never received from Subtask 4.7, so PI dropped loading condition as variable
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	Mar-14		Due date has been revised to reflect status of expts.
	Complete thermophysical & geomechanical property data analysis & validation	Apr-14		Due date has been revised to reflect status of expts.

<b>ID</b>	<b>Title/Description</b>	<b>Planned Completion Date</b>	<b>Actual Completion Date</b>	<b>Milestone Status</b>
4.8	Developing a predictive geologic model of the Green River oil shale, Uinta Basin			
	Detailed sedimentologic & stratigraphic analysis of three cores &, if time permits, a fourth core	Dec-12	Dec-12	Discussed Jan. 2013 quarterly report
	Detailed mineralogic & geochemical analysis of same cores	Dec-12	Dec-12	Discussed Jan. 2013 quarterly report
4.9	Experimental characterization of oil shales & kerogens			
	Characterization of bitumen and kerogen samples from standard core	Jan-12	Feb-12	Email sent to R. Vagnetti on Feb. 6, 2012 & discussed in April 2012 quarterly report
	Development of a structural model of kerogen & bitumen	Jun-12	Jun-12	Discussed in July 2012 quarterly report
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	Dec-12	Submitted with Jan. 2103 quarterly report
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-12	Aug-13	All models/data have been uploaded to the ICSE website

<b>ID</b>	<b>Title/Description</b>	<b>Planned Completion Date</b>	<b>Actual Completion Date</b>	<b>Milestone Status</b>
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			
	Make experimental recommendations	Aug-13	Aug-13	Discussed in this quarterly report
	Infer permeability-porosity-temperature relationships, develop model that can be used by other subtasks	Jan-14		Due date has been revised to reflect status of expts.
	Basic reservoir simulations to account for thermal front propagation	Aug-14		Due date has been revised to reflect status of expts.
	Evaluation of flow mechanics	Aug-14		Due date has been revised to reflect status of expts.
7.2	Kinetic compositional models & thermal reservoir simulators			Project has been terminated
	Incorporate chemical kinetics into thermal reservoir simulators	Jun-12	Jun-12	Discussed in July 2012 quarterly report
7.3	Rubblized bed HPC simulations			
	Collect background knowledge from AMSO about characteristics & operation of heated wells	Jun-12	Jun-12	Discussed in July 2102 quarterly report
	Perform generation 1 simulation - DEM, CFD & thermal analysis of characteristic section of AMSO rubblized bed	Sep-12	Sep-12	Discussed in Oct. 2012 quarterly report
	Perform generation 2 simulation that incorporates kinetic compositional models from subtask 7.2 and/or AMSO	Jun-13	Jan-14	Delayed due to priorities of AMSO

## NOTEWORTHY ACCOMPLISHMENTS

Subtask 4.7 and 7.1 researchers have overcome initial equipment commissioning issues and quality data are being generated. They are developing material response curves encompassing temperature, confining pressure and grade.

## PROBLEMS OR DELAYS

With the approval of a no-cost extension and the pending request for rebudgeting among several of the projects, several project milestones and deliverables have been revised, including those for Subtasks 3.2, 4.2, 4.3, 4.7, 4.8, 4.9, 7.1, and 7.3. The Subtask 4.7 experimental program at high temperature has been challenging, but the vessel is now functional under uniaxial compression. Upcoming tests will be triaxial, meaning that the confining pressure system will need to be debugged. The separator/condensation system will also need to be tested. The completion of Subtask 4.8 has been delayed due to health issues of the graduate student working on the project.

## RECENT AND UPCOMING PRESENTATIONS/PUBLICATIONS

- Bauman, J. H. & Deo, M. D. (2012). Simulation of a conceptualized combined pyrolysis, in situ combustion, and CO<sub>2</sub> storage strategy for fuel production from Green River oil shale. *Energy and Fuels*, 26, 1731-1739.
- Vanden Berg, M. D., Birgenheier, L. P. & Rosenberg M. J. (2012, September). Core-based sedimentologic, stratigraphic, and geochemical analysis of the lacustrine upper Green River Formation, Uinta Basin, Utah: Implications for conventional and unconventional petroleum development. Paper presented at the 2012 American Association of Petroleum Geologists - Rocky Mountain Section Meeting, Grand Junction, CO.
- Rosenberg, M.J., Birgenheier, L.P. & Vanden Berg, M.D. (2012, October). Sedimentology and sequence stratigraphy of the Green River Formation, eastern Uinta Basin, Utah. Paper presented at the 32<sup>nd</sup> Oil Shale Symposium, Golden, CO, October 15-19, 2013.
- Burnham, A., Day, R., Switzer, L., McConaghy, J., Hradisky, M., Coates, D., Smith, P., Foulkes, J., La Brecque, D., Allix, P., Wallman, H. (2012, October). Initial results of the AMSO RD&D pilot test program. Paper presented at the 32<sup>nd</sup> Oil Shale Symposium, Golden, CO, October 15-19, 2013.
- Deo, M. (2012, October). *Oil shale liquefaction: Modeling and reservoir simulation*. Short course presentation to Statoil, Trondheim, Norway.
- Deo, M. (2012, October). *Oil shale conversion to liquids: Experimental aspect*. Short course presentation to Statoil, Trondheim, Norway.
- Fletcher, T. H. (2012, October). *Oil shale 1: Chemical structure and pyrolysis*. Short course presentation to Statoil, Trondheim, Norway.
- McLennan, J. (2012, October). *Legacy and new geomechanical measurements of oil shale*. Short course presentation to Statoil, Trondheim, Norway.
- Smith, P. J. (2012, October). *Multiscale simulation*. Short course presentation to Statoil, Trondheim, Norway.

- Smith, P. J. (2012, October). *A description of a UQ-predictive validation framework for application to difficult engineering problems*. Short course presentation to Statoil, Trondheim, Norway.
- Tiwari, P., Deo, M., Lin C. L. & Miller, J.D. (2012, October). Characterization of the oil shale core pore structure before and after pyrolysis. Paper presented at the 2012 AIChE Annual Meeting, Pittsburgh, PA, October 28-November 2, 2012.
- 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. (2012). Three-dimensional structure of the Siskin Green River oil shale kerogen model: A comparison between calculated and observed properties. *Energy and Fuels*, 27, 702-710.
- Spinti, J. (2013, January 10). Presenter/panelist - *The real impact of oil shale and oil sands development in Utah*. 2013 Governor's Energy Development Summit, Salt Lake City, UT.
- Hradisky, M., Smith, P. J. & Burnham, A. (2013, March). *STAR-CCM+ simulations of in-situ thermal treatment of oil shale*. Paper presented at the STAR Global Conference, Orlando, FL, March 18-20, 2013.
- Orendt, A. M., Solum, M. S., Facelli, J. C., Pugmire, R. J., Chapman, K. W., Winans, R. E. & Chupas, P. (2013, April). Characterization of shale and kerogen from a Green River oil shale core, ENFL-535. Paper presented at the 245<sup>th</sup> American Chemical Society National Meeting, New Orleans, LA, April 7-11, 2013.
- Birgenheier, L. P. (2013, May 7). Presenter/panelist - *Constructing a basin-wide geologic model*. University of Utah Unconventional Fuels Conference, Salt Lake City, UT.
- Smith, P. J. (2013, May 7). Presenter/panelist - *Simulation of in situ production process using computational fluid dynamics*. University of Utah Unconventional Fuels Conference, Salt Lake City, UT.
- Spinti, J. P. (2013, May 7). Presenter/panelist - *Assessment of unconventional fuels development costs*. University of Utah Unconventional Fuels Conference, Salt Lake City, UT.
- Birgenheier, L.P., Plink-Bjorklund, P., Vanden Berg, M.D., Rosenberg, M., Toms, L. & Golab, J. (2013). *A genetic stratigraphic framework of the Green River Formation, Uinta Basin, Utah: The impact of climatic controls on lake evolution*. Paper presented at the American Association of Petroleum Geologists Annual Meeting, Pittsburgh, PA, May 22-25, 2013.
- Vanden Berg, M. D., Eby, D. E., Chidsey, T. C. & Laine, M.D. (2013). *Microbial carbonates in cores from the Tertiary (Eocene) Green River Formation, Uinta Basin, Utah, U.S.A.: Analogues for non-marine microbialite oil reservoirs worldwide*. Paper presented at Microbial Carbonates in Space and Time: Implications for Global Exploration and Production, The Geological Society, London, United Kingdom, June 19-20, 2013.
- Rosenberg, M. J. (2013). Facies, stratigraphic architecture, and lake evolution of the oil shale bearing Green River Formations, eastern Uinta Basin, Utah. M.S. thesis, Department of Geology and Geophysics, University of Utah.
- Tiwari, P., Deo, M., Lin, C. L. & Miller, J.D. (2013, May). Characterization of oil shale pore structure before and after pyrolysis by using X-ray micro CT. *Fuel*, 107, 547-554.

- Pugmire, R. J., Fletcher, T. H., Hillier, J., Solum, M., Mayne, C. & Orendt, A. (2013, October). Detailed characterization and pyrolysis of shale, kerogen, kerogen chars, bitumen, and light gases from a Green River oil shale core. Paper presented at the 33<sup>rd</sup> Oil Shale Symposium, Golden, CO, October 14-16, 2013.
- Fletcher, T. H., Gillis, R., Adams, J., Hall, T., Mayne, C. L., Solum, M.S. & Pugmire, R. J. (2013, October). Characterization of pyrolysis products from a Utah Green River oil shale by <sup>13</sup>C NMR, GC/MS, and FTIR. Paper presented at the 33<sup>rd</sup> Oil Shale Symposium, Golden, CO, October 14-16, 2013.
- Wilkey, J., Spinti, J., Ring, T., Hogue, M. & Kelly, K. (2013, October). Economic assessment of oil shale development scenarios in the Uinta Basin. Paper presented at the 33<sup>rd</sup> Oil Shale Symposium, Golden, CO, October 14-16, 2013.
- Hillier, J. L., Fletcher, T. H., Solum, M. S. & Pugmire, R. J. (2013, October). Characterization of macromolecular structure of pyrolysis products from a Colorado Green River oil shale. Accepted, *Industrial and Engineering Chemistry Research*. dx.doi.org/10.1021/ie402070s
- Birgenheier, L. & Vanden Berg, M. (n.d.). Facies, stratigraphic architecture, and lake evolution of the oil shale bearing Green River Formation, eastern Uinta Basin, Utah. To be published in Smith, M. and Gierlowski-Kordesch, E. (Eds.). *Stratigraphy and limnogeology of the Eocene Green River Formation*, Springer.
- Solum, M. S., Mayne, C. L., Orendt, A. M., Pugmire, R. J., Hall, T., Fletcher, T. H. (2013). Characterization of macromolecular structure elements from a Green River oil shale-(I. Extracts). Submitted to *Energy and Fuels*, September, 2013.
- Kelly, K.E., Wilkey, J. E. Spinti, J. P., Ring, T. A. & Pershing, D. W. (2013). Oxyfiring with CO<sub>2</sub> capture to meet low-carbon fuel standards for unconventional fuels from Utah. Submitted to *International Journal of Greenhouse Gas Control*, October, 2013.
- Fletcher, T. H., Gillis, R., Adams, J., Hall, T., Mayne, C. L., Solum, M.S., and Pugmire, R. J. (n.d.). Characterization of pyrolysis products from a Utah Green River oil shale by <sup>13</sup>C NMR, GC/MS, and FTIR. Manuscript in preparation.

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## **APPENDIX A. Abstracts for Presentations at the 33rd Oil Shale Symposium, Golden, Colorado, October 14-16, 2013**

### **1. Detailed Characterization and Pyrolysis of Shale, Kerogen, Kerogen Chars, Bitumen, and Light Gases from a Green River Oil Shale Core**

Ronald Pugmire<sup>1</sup>, Thomas Fletcher<sup>2</sup>, James Hillier<sup>2</sup>, Mark Solum<sup>1</sup>, Charles Mayne<sup>1</sup>, Anita Orendt<sup>1</sup>

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The Utah Geological Survey (UGS) and the University of Utah Institute for Clean and Secure Energy, as part of its oil shale program, drilled a 1000 foot core at the Uinta Skyline 16 location. This core provided the oil shale program with a well-defined, well-controlled, fresh, moisture protected sample on which to obtain a consistent set of data on both the chemical and geological nature of both the shale and the isolated kerogen. UGS and the Energy & Geoscience Institute logged the core samples properties at different depths. Three one-foot segments of this core were chosen to be carefully studied (461.1-462.1, 484.9-486.9, and 548.1-549.1). These one foot core samples were ground and sized for further analytical analysis. Detailed analytical characterization was obtained on each of the shales, the isolated kerogen, as well as the kerogen pyrolysis products (char, bitumen, and light gases obtained at various pyrolysis temperatures). The shale, isolated kerogen, and kerogen chars (over a wide temperature range) were studied by solid state carbon-13 NMR by both one- and two-dimensional techniques and the structural details of these samples were determined following the same procedures developed at the University of Utah to obtain detailed molecular structure components of coal and coal derived products. The methylene soluble bitumen samples were studied by means of both proton and carbon-13 NMR techniques. The GC/MS data obtained on the tar samples were also highly informative and complemented the liquid proton and carbon-13 NMR data. Analysis of the light gases released at the various pyrolysis temperatures provides additional detail of the transformations of the kerogen structures. The structural details obtained in this study are complemented by utilizing experimental data obtained at the Advanced Photon Source at Argonne National Laboratory. Measurement of the atomic pair distribution function (PDF) for a powdered (100 mesh) kerogen sample, together with advanced computational computing resources at the University of Utah, allowed a 3-D model to be developed that contains an average structure of this Green River kerogen.

### **2. Characterization of Pyrolysis Products from a Utah Green River Oil Shale Sample by 13 C NMR, GC/MS, and FTIR**

Thomas H. Fletcher<sup>1</sup>, Ryan Gillis<sup>1</sup>, Jacob Adams<sup>1</sup>, Charles L. Mayne<sup>2</sup>, Mark S. Solum<sup>2</sup>, Ronald J. Pugmire<sup>2</sup>

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Three samples of oil shale from the Green River Formation in Utah were demineralized, and the resulting kerogen was pyrolyzed at 10K/min at atmospheric pressure in nitrogen for temperatures up to 525°C. The pyrolysis products (light gas, tar, and char), where tar is defined as the condensable gas and char defined as the solid residue remaining, were analyzed using 13C NMR, GC/MS, and FTIR. Low temperature ashing was performed in order to compare pyrolysis yields of oil shale and demineralized kerogen on a dry ash-free (DAF) basis. Pyrolysis yields of 80% dry ash-free basis were achieved at these conditions, with 60% DAF tar yield at the highest temperature. The solid-state NMR results indicate that the aromaticity of the kerogen char increased from 20% to 80% during pyrolysis, with a

corresponding decrease in the average aliphatic carbon chain length from 12 to less than one. The average number of aromatic carbons per cluster increased from 12 to 20 in a narrow temperature window between 425 and 525°C, with an increase in the number of attachments per cluster from 6 to 8 in that same temperature window. Liquid-state NMR results of the condensed tars showed a predominance of n-alkyl chains, with similar carbon aromaticities at each temperature. The alkyl chains were also observed in the GC/MS data. The light gases determined by FTIR were primarily CH<sub>4</sub>, CO, and CO<sub>2</sub>. The combination of gas, tar, and char yields and product analyses are valuable data for modelling of oil shale processes.

### 3. Economic Assessment of Oil Shale Development Scenarios in the Uinta Basin,

Jonathan Wilkey, Jennifer Spinti, Terry Ring, Michael Hogue, Kerry Kelly

University of Utah, Salt Lake City, UT, USA

The enormous size of U.S. oil shale resources in general, and Utah resources in particular, is well-known. However to date there has been no commercial scale production of liquid transportation fuels from oil shale in the U.S. despite the size of the resource and demonstrations of the technical feasibility of various production methods. What is constraining development? This study seeks to answer this question by assessing the economic feasibility of a 50,000 BPD oil shale facility in Utah's Uinta Basin under various production scenarios. The scenarios encompass extraction of raw shale oil (by ex situ or in situ methods), upgrading to a light low-sulfur synthetic crude oil, and transportation via pipeline from the Uinta Basin to refineries in North Salt Lake City, UT. A discounted cash flow analysis is performed to find the net present value, rate of return, and required oil price for each scenario, based on each scenario's capital and operating costs as determined by their mass and energy balances. Additionally, a detailed breakdown of all costs, material, and energy requirements for each scenario are presented on a per barrel basis. Finally, the sensitivity of each production scenario to various parameters, such as higher or lower capital and operating costs, tax and royalty rates, and CO<sub>2</sub> policies (carbon tax and oxy-firing for carbon capture) are considered and their cost impacts are quantified. For the production methods analysed, capital costs were estimated to be on the order of \$5-\$6 billion dollars (for both ex situ and in situ extraction methods). Ex situ methods were found to break even at \$76-\$78 per barrel (depending on the retorting method), resulting in a 10% internal rate of return under U.S. Energy Information Administration reference oil price forecasts. The in situ extraction method modelled here performs much worse economically because of the long delay between heating and production, resulting in a break-even price of \$183 per barrel.

### 4. High Performance Computing Simulations of In-situ Thermal Treatment of Oil Shale

Michal Hradisky<sup>1</sup>, Philip Smith<sup>1</sup>, Alan Burnham<sup>2</sup>

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<sup>2</sup>American Shale Oil, LLC, Rifle, CO, USA

One of the many research areas at the University of Utah Institute for Clean and Secure Energy is to assist in the commercial utilization of the vast energy stored in domestic oil shale and oil sands resources. We are exploring in-situ thermal treatment technologies of oil shale development because of their potential for reducing environmental footprints. We are taking the novel approach of applying High Performance Computing (HPC) using STAR-CCM+ and Validation and Uncertainty Quantification (V/UQ) to perform Computational Fluid Dynamics (CFD)-based simulations to quantitatively predict performance of in-situ thermal heating process of oil shale. We are closely working with American Shale Oil (AMSO) corporation and

performing simulations of their process located in Rifle, CO. In many oil shale applications the rate limiting step is the rate of heat transfer in the thermal treatment process. Using HPC STAR-CCM+ simulations, we are able to monitor the temperature evolution and distribution inside the formation and quantify uncertainties associated with thermal diffusion for their heater test.

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