Oil & Natural Gas Technology

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

Quarterly Progress Report (October – December 2009)

Submitted by: Institute for Clean and Secure Energy 155 S. 1452 E. 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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Principal Investigator: Philip J. Smith Project Period: October 1, 2009 to March 31, 2011

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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. The program was officially launched on October 1, 2009. The project management plan was submitted for review in November 2009 and has now been finalized. In this guarter, the Clean and Secure Energy program focused on enhancing its dialogue with industry. Seminars presented by the Itasca Group and Red Leaf Resources were sponsored by ICSE as was a field trip to Enshale's oil shale demonstration plant south of Vernal, Utah. Significant efforts were also made in this guarter to enhance other ICSE outreach tools, including the repository, the interactive map, and the website. New private collections have been added to the repository to facilitate communication among ICSE researchers. A new public collection containing peer-reviewed ICSE Research Publications has also been established. The interactive map is being augmented with water-related data. Work at the Utah Geological Survey on the thickness and richness of oil shale zones will further enhance the value of the map. In Task 3.0, ICSE researchers have begun gathering literature data on the potential of oxyfuel for CO₂ capture in refining and oil sands upgrading operations and have computed preliminary estimates of life-cycle well-to-pump CO₂ emissions for crude oil refining under both baseline and improved process-heater efficiency conditions. In addition, researchers have set up a simulation test matrix based on experimental work performed in a oxy-gas fired furnace at the International Flame Research Foundation. This test matrix considers the impact of fuel/ oxidant inlet velocities, chemistry/mixing model, and mesh resolution on axial velocity and gas composition in the furnace. In Task 4.0, ICSE researchers are focused on the vertical integration of all subtasks into an overarching simulation that considers liquid fuel production from the insitu thermal treatment of oil shale/sands. To achieve this integration, they are planning to use standard samples and a handling protocol. The Subtask 4.1 team has been formulating a theoretical approach to modeling in-situ heating of oil shale and oil sands. This approach will be implemented in the Arches LES code to model the Red Leaf ECOSHALE capsule. Geometry information has been obtained from Red Leaf with additional information to follow. The Subtask 4.2 team focused on using experimental design techniques to identify model parameters that most influenced the ultimate recovery of oil from an in-situ oil shale pyrolysis scenario. The kerogen cracking activation energy, the relative permeability representation, the oil cracking to gas activation energy, and possibly the activation energy distribution representation were found to have significant impacts on the ultimate recovery of oil in these simulations. Researchers in Subtask 4.3 used TGA analysis to identify the differences the weight loss and reaction kinetics of oil shale in three different sweep gas environments (nitrogen, air and CO₂). For all three environments, the decomposition temperature range shifted to higher temperatures as the heating rate increased. The Subtask 4.4 team compared TGA decomposition data of dry shale and samples soaked in water for five months. The peak decomposition temperatures of watersoaked samples were slightly higher than the baseline samples. A pyrolyzed oil shale sample subjected to X-ray nano tomography by the Subtask 4.5 team exhibited two distinct regions of cracks and voids. The estimated permeability from Lattice Boltzmann simulations of this pyrolyzed sample was 0.363 mD. ICSE researchers in Subtask 4.6 determined that their 12-unit kerogen model had some deficiencies. They modified their models to reflect certain degrees of cross-linking in the structures to mimic published data from oxidation experiments. In Task 5.0, ICSE researchers continued to monitor and review (1) litigation challenging the federal oil shale leasing rule and the Programatic EIS for oil shale and oil sands leasing and (2) rulemaking and research relating to water resources and water quality. Lastly, in Task 6.0, the research team developed a plan for the process flow sheets needed for the various scenarios, continued research related to environmental and greenhouse gas regulatory issues and externalities associated with the Canadian oil sands production, developed criteria for refining the scenarios on which to perform a supply cost analysis, and continued work on the revenue side of the viability issue.

PROGRESS, RESULTS, AND DISCUSSION

Task 1.0 - Project Management and Planning

The project management plan (PMP) had a scheduled completion date of November 2009. A draft version of the PMP was submitted to NETL in early November. A revised version of the PMP, incorporating NETL feedback, was submitted in late December 2009.

Task 2.0 -Technology Transfer and Outreach

This task is focused on (1) enhancing the dialogue between ICSE and industry and (2) engaging in academic and public outreach/education efforts. To accomplish these goals, ICSE sponsored several field trips, industrial seminars, and academic presentations during this guarter. In October, Dr. Marisela Sanchez from the Itasca Group gave a geomechanics seminar addressing issues associated with in situ production of unconventional fuels (how permeability changes with stress, coupling geomechanics with reservoir simulation, etc.). The Itasca Group is an international engineering consulting and software development firm that specializes in geomechanics-related problems. Three events were held in November. First, ICSE hosted a group of visitors from Los Alamos National Laboratory headed by Dr. Andy Wolfsberg. Dr. Wolfsberg's group is interested in collaboration with ICSE to further the development and utility of their Climate-Energy Assessment for Resiliency (CLEAR) model. They are specifically interested the use of the CLEAR model in Subtask 3.1 and in the scenarios, models, and data collected for Subtask 6.3. Second, Dr. James Bunger from Red Leaf Resources presented an ISCE seminar on the Ecoshale process. Third, Professor Ron Pugmire, a faculty member in ICSE, presented a seminar entitled "13C NMR Spectroscopy: A Key Contributor for Development of the Molecular Structure of Coal and Other Kerogens." The presentation was videotaped as is available for download from the ICSE repository. Two events were held in December. One, a small group of ICSE faculty, staff, and students drove to the Uinta Basin, Utah, for a tour of the Enshale plant. Enshale, a subsidiary of Bullion Monarch Mining, is conducting tests of an indirect retorting technology at their demonstration plant south of Vernal, Utah. Two, Professor John McClennan, a faculty member affiliated with ICSE and with the Energy and Geoscience Institute, presented a seminar entitled "Introduction to Oil and Gas: Drilling and Completion Overview."

Other major outreach activities during this guarter include the continued expansion of the ICSE repository and interactive map and the development of a new ICSE website. The ICSE repository uses the DSpace software platform to archive materials related to oil shale and oil sands for use by ICSE researchers and by the broader unconventional fuels community. There are two communities in ICSE, a private community and a public community. The Institute Librarian, Wendy Ajax, has continued to work with administrators of the private DSpace collections and has begun to review and cull these collections for documents that can be added to the public DSpace community. Work has also begun on gathering publications of ICSE researchers and reviewing copyright issues associated with uploading those publications to the public DSpace community. In addition, new web pages, search options and a new collection were added for the ICSE Research Publications collection. This collection will house documents published by ICSE after a peer-review process. The ICSE Web Applications Programmer, Terrance Davis, began the migration conversion of DSpace needed to support the database migration from Oracle to Postgresgl. Further, DSpace modifications were made to improve general searching and browsing of the public community. DSpace login and post-login menus were also revised to be more accessible and user-friendly for general users of the repository.

For the ICSE interactive map, feedback was collected from several beta testers. This feedback was very constructive and will help guide map activities in the upcoming quarters. Additionally, the ICSE GIS Applications Developer, Michelle Kline, began adding geospatial water datasets. Dataset review and refinement will continue until the completion of the project task, as will contemporaneous inclusion of these datasets in the project map server. The ICSE interactive map was presented and demonstrated at the 29th Oil Shale Symposium in Golden, Colorado.

An additional effort related to the map is the validation of the White River water management model and the demonstration of a water management geodatabase and model for assessing impacts of climate variability on White River streamflows and its ability to meet water demands estimated for future oil shale development. This work is being coordinated with the Utah Division of Water Resources to assess climate variability impacts on White River flows and the implications for potential energy development in the Uinta Basin. Data describing the proposed White River reservoir characteristics have been incorporated into the geodatabase and water management model, and an analysis is currently being completed assessing the feasibility of the reservoir in response to hydrologic cycle changes associated with climate variability. When this work is complete, the geodatabase will be uploaded to the interactive map.

A third effort with the interactive map is being carried out by Michael Vanden Berg and colleagues at the Utah Geological Survey. This effort is focused on providing the thickness and richness of each oil shale zone in the Uinta Basin, Utah. In this quarter, the project team calculated the richness of oil shale zones in ~340 wells from the Uinta Basin, Utah, including the R-8, A-groove, Mahogany, B-groove, Upper R-6, Mid/Lower R-6, L-5, R-5, L-4, R-4, and R-8 through R-4 zones. The team also began construction of isopach maps representing the richness of each zone.

Finally, significant work was completed on developing a more integrated ICSE website. The new website, to be rolled out in the first quarter of 2010, will have improved links to research projects, the ICSE repository and interactive map, and the calendar of events.

Task 3.0 - Clean Oil Shale and Oil Sands Utilization with CO₂ Management

Subtask 3.1 – Macroscale CO₂ Analysis

During this quarter, the project team began gathering literature data on process heaters, oxyfuel process heaters, oxy-fuel flameless process heaters, and the potential of oxy-fuel for CO₂ capture in refining and oil sands upgrading operations. Because more information is available for refining operations than for oil sands upgrading, the initial analyses will focus on refining.

The United States refining industry consumes approximately $1.4 - 2.2 \times 10^{15}$ BTU/yr in process heaters, and the average efficiency of these heaters ranges from 75-80%. For most process heaters, an efficiency improvement of 10% is feasible with air preheat and improved burner design (DOE, 2004; DOE, 2006), although flameless combustion can provide additional efficiency improvements. Figure 1 provides life-cycle well-to-pump CO₂ emission estimates for refining of crude oil under baseline conditions and with improved process-heater efficiency. These preliminary CO₂ estimates assume that the fuel saved in the process heaters is the same as for refining in general. This assumption is being evaluated.



Figure 1: Life-cycle well-to-pump CO₂ emissions per MJ of gasoline produced in a refinery with conventional-efficiency process heaters and improved-efficiency process heaters. The baseline life-cycle CO₂ emissions were obtained from Argonne National Laboratory's GREET model.

The investigators are also beginning to evaluate existing tools for determining life-cycle emissions from transportation fuels, such as GREET and GHGenius (S&T Consultants), and the relevant systems models, such as the CLEAR model (Los Alamos National Laboratory).

Subtask 3.2 - Flameless Oxy-gas Process Heaters for Efficient CO2 Capture

The project team has selected the International Flame Research Foundation's (IFRF) oxy-gas experiments as the foundation for their verification/uncertainty quantification analysis. These datasets, known as the OXYFLAM experiments, were collected in 1995-1996 in the IFRF Furnace No. 2 as shown Figure 2 (Lallement et al., 1997). The furnace consists of 13 segments with a length of 0.3 m each and a cross section of 1.2x1.2 m. In one set of experiments, the furnace walls were water-cooled while in a second set of experiments, the furnace walls were lined with refractory. Three oxy-natural gas burners based on the same generic, double pipe design (see Figure 3) were used. The variable in the burner design was the diameter of the pipes, leading to high, medium, and low momentum burners.



Figure 2: Configuration of IFRF Furnace No. 2 for OXYFLAM experiments (Lallement et al., 1997).



Figure 3: Generic burner used in OXYFLAM experiments (Lallement et al., 1997).

From a simulation standpoint, the simple geometry of both the furnace and the burner makes the case ideal for the Arches LES code. A case was set up with the furnace walls as the domain boundary condition and the furnace interior as the computational domain. Arches was designed for systems with open boundary conditions (e.g. no walls), so some code development/ debugging has been necessary to run this particular configuration.

Also in this quarter, an experimental design was proposed. The purpose of the experimental design is to probe the parameter space that has the greatest effect on the response quantity of interest (e.g. posterior). In the case of the IFRF data, the following measurements were taken: wall temperature, gas temperature, gas composition, soot concentration, total radiance, total radiative flux at the wall, furnace heat extraction, axial velocity, and turbulence intensity. In oxy-gas combustions systems, the questions most often asked relate to how oxy-gas firing changes the local temperature, the local gas composition, and the radiant heat transfer. However, before choosing these data as the response quantities of interest, one must consider the reported experimental error for the various types of measurements taken. The authors in the IFRF report expressed most confidence in the accuracy of the velocity data. The gas temperature data were off by several hundred degrees but could be corrected with some confidence using a calibration curve given in the report. The gas composition data may have been affected by recombination

reactions in the sampling probe, particularly the H2 concentration which may be a few percent high. Radiation measurements were hampered by the lack of a blackbody at a calibration temperature high enough (1650°C) for the refractory-lined furnace (Lallemant et al., 1997). For these reasons, the V/UQ analysis will focus on first, the velocity data and second, the composition data. The radiation data may also be considered if there is time.

Parameter selection for the experimental design is focused on those numerical, boundary condition, or model errors that most influence the velocity and gas composition (and potentially the radiation). From previous research (Nguyen, 2009), the project team knows that the inlet flowrates of both fuel and oxidant can have a strong effect on the velocity field. It should be noted that the IFRF report comments that the fuel and oxidant flow rates were hard to control (Lallemant et al., 1997). This effect can be modeled either by changing the range of inlet flowrates of the two streams or changing the burner geometry to reduce the inlet velocity. The composition field is affected by the choice of chemistry/mixing model. The fidelity of the simulation results will depend on whether or not the relevant time/length scales are captured by the chosen for the experimental design: burner geometry, chemistry/mixing model, and mesh resolution.

In past work, the project team has used a Box-Behnken experimental design to generate a response surface relating the three priors to the response quantity of interest (e.g. posterior). However, because the Box-Behnken design is not intended for predicting a response at extremes (e.g. edges of the parameter space being probed), a Face-Centered Composite Design (FCC), which samples the design space at the extrema, will be implemented for this project (NIST, 2010). Figure 4 shows qualitatively the differences in the design spaces for both designs. For a three-parameter design, 16 simulation runs are required.



Figure 4: Box-Behnken (left-hand side) and Face-Centered Composite (right-hand side) Design spaces (Myers and Montgomery, 1995).

With the choice of chemistry/mixing model as a prior, the incorporation of qualitative priors, priors to which the concept of continuity does not apply, needs to be addressed. The effect of these qualitative priors on the posterior must be captured. If one assumes that there is no interaction between qualitative priors and the posterior(s), this problem can be simplified

enormously. The coefficients of the interaction terms are zero and only the linear terms of the qualitative variables are needed in the model. In other words, in the proposed design, the project team has assumed that if the chemistry/mixing model is changed from an equilibrium model to a flamelets model, the equation for the response surface will only change by a constant with the other coefficients staying the same.

The FCC design typically involves 3 evenly-spaced levels (low, medium, and high) of each parameter. The parameters are assumed to be continuous. Because the chemistry/mixing model variable does not meet this criteria, a modified FCC design is proposed that will provide the same information as a normal FCC design while simultaneously accommodating the discrete variables. The first and last parameters, burner design and domain resolution, are "continuous." The second parameter, chemistry/mixing model, is a discrete parameter but will be treated as a continuous variable in the design. After the response surface is created, this parameter will be fixed at one of the three levels. The three parameters chosen, together with the corresponding low, medium, and high levels, are listed below:

- Burner Design [A, B, C]
- Chemistry/Mixing Model = [Equilibrium_Clipped Gaussian, Flamelets_Delta, Flamelets_Clipped Gaussian]
- Domain Resolution [120, 180, 240]

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

All ICSE researchers involved in the various subtasks meet on a monthly basis to discuss progress, identify connections, and address issues of concern. In meetings this quarter, the task team has defined a series of standard samples, handling protocols and spectroscopic measurements that will be used to guide the simulation/modeling work.

<u>Subtask 4.1 - Development of CFD-based Simulation Tools for In-situ Thermal Processing of Oil</u> <u>Shale/Sands</u>

The ultimate goal of this subtask is to perform a validation/uncertainty quantification analysis of the Red Leaf ECOSHALE test capsule. To perform such an analysis, high quality experimental data is required. During this quarter, Red Leaf conducted an autopsy of their ECOSHALE test capsule. The autopsy consisted of drilling several core holes into the capsule, both in the shale bed and in the Flexcrete wall. ICSE researchers met with Red Leaf personnel several times and advised them on the location of core holes to drill and the types of tests that could be conducted on the resulting samples. Suggested tests included extractions, thermogravimetric analysis (TGA), pyrolysis, Fischer assay, simulated distillation of the oil, and elemental analyses of the oil for the purpose of answering questions about the location of extractable oil, the production potential of the spent shale, and the composition of the produced oil. ICSE researchers also received information on the capsule dimensions.

In order to perform a simulation of the ECOSHALE capsule, the Arches LES simulation tool, developed by ICSE researchers, needs to be modified to accommodate flow through a porous bed. The theoretical approach to modeling in-situ heating of oil shale and oil sands is being formulated. The gas phase flow field will be modeled by tracking porosity and permeability. The permeability can be represented by up to 9 scalars, as it is treated as a tensor. These variables will be tracked using the direct quadrature method of moments (DQMOM) and will require models for their temporal evolution. In addition, models for the temporal evolution of other distributions of interest, namely temperature and oil content, are also required, as these variables will also be tracked using DQMOM. A kinetic model for oil shale pyrolysis is still in the

process of selection; these model equations will be incorporated into the Arches code once complete.

Subtask 4.2 - Basin-wide Characterization of Oil Shale Resource in Utah and Examination of Insitu Production Models

The project team focused this quarter on which model parameters most influence the ultimate recovery of oil in in-situ oil shale pyrolysis simulations. The relative permeability representation, the molecular representation of organic components, and kinetic parameters are potentially such parameters. Experimental design and analysis techniques were used to determine the impact of these parameters on the ultimate recovery of oil and their fundamental relationships with each other. By identifying parameters supplied to governing equations and theoretical models that have the greatest impact on the final recovery of oil predicted, the project team can focus its efforts on improving the accuracy of those parameters. Some of the material in this quarterly report (Table I, Table IV, and Figure 8) was reported in a previous phase of the project but is included here for completeness.

For the simulations described in this report, STARS, a thermal reservoir simulator created by CMG, was used. In these simulations, vertical heating wells surround a producer in a seven point pattern. Only a triangular wedge with fractions of 2 heaters and a fraction of 1 producer is discretized and calculated as shown in Figure 5. The initial dimensions of the wedge were 53 feet between heaters and 50 feet thickness of the reservoir. The temperature at the heating wells was quickly raised to approximately 800°C and then controlled at about 650°C in order to supply sufficient heat for adequate heat transfer throughout the reservoir and to maintain reasonable temperatures near the heating well. Geological data from the Mahogany zone in the Uinta Basin well U059 was used to estimate the richness of the layers in the reservoir. The richness of the layers varies from 12.5 – 25 wt% of hydrocarbon material in the oil shale. All of the hydrocarbons were assumed to be kerogen, and this kerogen was assumed to occupy 90-95% of the pore space, the rest of the pore space being occupied with 99% methane and 1% water. Kerogen was specified with a constant solid density, so rich layers were assigned higher porosities and lean layers were assigned lower porosities. Horizontal permeability varied from 0.1 mD (millidarcy) at the bottom of the reservoir to 1 mD at the top and vertical permeability varied from 0.05 mD at the bottom of the reservoir to 0.5 mD at the top.

It is likely that a permeability creation/destruction model will be necessary to model this process due to solid kerogen conversion to fluids, volume expansion of the rock, and coke plugging of pores. Since these geomechanical phenomena are little understood, they are neglected in this study.





A multi-step reaction scheme was used to estimate kerogen decomposition to products. All hydrocarbons were lumped into 7 representative components: kerogen, heavy oil, light oil, gas, methane, char, and coke. The reaction scheme was adapted from a previous study (Braun and Burnham, 1992) and is similar to other kerogen decomposition models (Stainforth, 2009), though the reaction scheme in this study is relatively simple.

- 1. Kerogen -> HO + LO + gas + CH4 + char
- 2. HO -> LO + gas + CH4 + char
- 3. LO -> gas + CH4 + char
- 4. gas -> CH4 + char
- 5. char -> CH4 + gas + coke

Experimental design and analysis methods are useful for comparing the responses due to variable input parameters, including their possibly significant interactions. The parameters of particular interest in this study are: (1) Molecular weight of kerogen/stoichiometry/initial kerogen molar concentration (these values are treated as one parameter since they are dependent on each other to conserve volume and mass balances), (2)-(5) activation energies for reactions 1-4, (6) with/without normal distribution of activation energies for reaction 1, (7) relative permeability representation, and (8) reaction enthalpy.

The molecular structure of kerogen is largely unknown. The molecular weight of kerogen has been reported in ranges from about 3,000 (Yen 1976) to 27,000 (Behar and Vandenbrouke 1987). Molecular weight ranges and the associated stoichiometry for reactions 1 and 2 are shown in Table I. The values in Table I demonstrate that stoichiometry for such a kinetic mechanism depends on the properties (molecular weight and H/C ratio) of the pseudo components and is therefore "non-unique." Mass and elemental balances are important in these representations.

Table I: High and low molecular weights and associated stoichiometry for reactions 1 and 2.

| | Kerogen | Heavy Oil | Light Oil | Gas | Methane | Char | coke |
|--------|----------|-----------|-----------|-------|---------|-------|-------|
| MW (+) | 20000.55 | 424.49 | 152.03 | 52.01 | 16.04 | 12.60 | 14.55 |
| MW (-) | 2974.84 | 424.61 | 151.99 | 51.95 | 16.04 | 12.55 | 14.55 |

| Form (+) | $C_{1479}H_{2220}$ | C _{31.75} H _{42.82} | C _{11.19} H _{17.51} | $C_{3.35}H_{11.63}$ | CH ₄ | CH _{0.55} | $C_{1.19}H_{0.32}$ |
|-----------------|-----------------------------------|---------------------------------------|---------------------------------------|--------------------------------------|-----------------|--------------------|--------------------|
| Form (-) | C ₂₂₀ H ₃₃₀ | C _{31.76} H _{42.81} | C _{11.19} H _{17.50} | C _{3.35} H _{11.62} | CH ₄ | CH _{0.53} | $C_{1.19}H_{0.32}$ |
| Stoic rxn 1 (+) | -1 | 37.29 | 13.86 | 25.03 | 17.06 | 38.71 | 0 |
| Stoic rxn 1 (-) | -1 | 5.55 | 2.06 | 3.72 | 2.54 | 5.8 | 0 |
| Stoic rxn 2 (+) | | -1 | 2.18 | 0.06 | 0.03 | 7.13 | 0 |
| Stoic rxn 2 (-) | | -1 | 2.18 | 0.06 | 0.03 | 7.13 | 0 |

Ranges for appropriate activation energies have been reported (Stainforth, 2009) and can vary significantly depending on experimental methods and analysis of results. These ranges for activation energy are shown in Table II.

Table II: Range of activation energies.

| Reaction | Low Activation Energy (kJ/mol) | High Activation Energy (kJ/mol) |
|--------------------|-----------------------------------|------------------------------------|
| Kerogen Cracking | 195 | 225 |
| Heavy Oil Cracking | 208 | 260 |
| Light Oil Cracking | 208 | 260/233 |
| Gas Cracking | 235 | 270 |

Studies have reported that activation energy for kerogen pyrolysis is most appropriately modeled with some distribution (Stainforth, 2009; Sundararaman, 1992), but it is uncertain how much impact different representations of activation energy have on the simulation results at large scales. A normal distribution with 5 kJ/mol standard deviation is shown in Figure 6. This energy distribution must be represented discretely in STARS. This discrete representation is determined by integrating under the distribution curve and then representing kerogen reacting at an appropriate activation energy.



Figure 6: Normal distribution of activation energies for reaction 1.

Relative permeability representations are often approximated in simulations, but such approximations may have significant implications. The range of representations are shown in Figure 7, the low value being more linear and the high value being curved.



Figure 7: Oil/water and liquid/gas relative permeability curves.

Efficient heat transfer through an oil shale reservoir is crucial to any successful operation. Heat of reaction for oil shale pyrolysis has been reported (Camp, 1987), but it is not certain how much heat is "lost" to reaction compared to heat required to raise the rock temperature.

The initial experimental design was a 2⁷⁻⁴ fractional factorial design. The eight-run design for the initial 7 factors (excluding (8) heat of reaction) is shown in Table III. Each row represents a simulation run at the parameter levels specified in the run. The un-coded levels for these parameters are shown in Table IV. Details about each of these parameters have been described above.

| Run | X1 | X2 | ХЗ | X4 | X5 | X6 | X7 |
|-----|----|----|----|----|----|----|----|
| 1 | - | - | - | + | + | + | - |
| 2 | + | - | - | - | - | + | + |
| 3 | - | + | - | - | + | - | + |
| 4 | + | + | - | + | - | - | - |
| 5 | - | - | + | + | - | - | + |
| 6 | + | - | + | - | + | - | - |
| 7 | - | + | + | - | - | + | - |
| 8 | + | + | + | + | + | + | + |

Table III: Eight run fractional factorial screening experimental design.

Table IV: Un-coded parameters for screening design.

| | | (-) | (+) |
|----|----------------|---------|--------|
| X1 | MW/stoic/conc. | 3000 | 20000 |
| X2 | E1 | 195 | 225 |
| Х3 | E2 | 208 | 260 |
| X4 | E3 | 208 | 260 |
| X5 | E4 | 235 | 270 |
| X6 | E distribution | without | with |
| X7 | rel perm | linear | curved |

The numerical performance for each of these runs was not equal. Some of the runs had excessive time step cuts due to rapid changes in gas saturation. The response chosen for these runs was simulation time in order to pinpoint the possible causes of these time step reductions. Figure 8 is a Pareto chart displaying the impact each of these parameters has on the simulation time. Activation energy for reaction 3, factor X4, had the greatest impact on the simulation time. After investigation, it appeared that simulation time increased significantly when the activation energy for reaction 3 was greater than the activation energy for reaction 4. This increase could be due to the combination of rapid gas creation coupled with high gas mobility causing rapid gas saturation changes. The high value for factor X4 was relaxed to 233 kJ/mol as shown in Table II, and no major differences in simulation time were observed in subsequent runs.



Figure 8: Pareto chart for parameter effects on simulation time.

Using the relaxed value for factor X4, runs in the fractional factorial design were completed with ultimate recovery of oil as the output response. None of the simulations produced acceptable amounts of oil. Oil generated from kerogen had inadequate mobility in lower temperature zones far from the heaters to flow to the producer. As a result, oil components had large residence times in the reservoir and eventually converted further to gas and residual components. The initial dimensions of the simulated domain were changed to assure that the whole reservoir was at a high enough temperature for adequate oil mobility. Figure 9 shows the modified dimensions of the simulated wedge with the distance between heaters being reduced from 53 ft to 26.5 ft.



Figure 9: Aerial view of simulated wedge. Distance between heating wells reduced to 26.5 ft.

The same fractional factorial design was used with ultimate recovery of oil as the response. The normal probability plot in Figure 10 illustrates the results of the runs. The fact that the plotted points are linear without outliers indicates that there is no evidence from these runs that any factors are dominant or insignificant. With a 2^{7-4} fractional factorial design, single factor effects are confounded with pair interaction effects and higher order interactions.



Figure 10: Normal probability plot of the effects on ultimate recovery of oil from 2⁷⁻⁴ fractional factorial design.

Further runs were done with a sixteen run fractional factorial design for 6 to 8 factors. All 8 factors, including heat of reaction, were tested with this design. The design used is shown in Table V. Factors E1 - E7 represent possible interactions between parameters, but individual factors are isolated from possible confounding with interactions.

| Run | Mean | X1 | X2 | Х3 | X4 | X5 | X6 | Х7 | X8 | E1 | E2 | E3 | E4 | E5 | E6 | E7 |
|-----|------|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|
| 1 | + | - | - | - | - | - | - | - | - | + | + | + | + | + | + | + |
| 2 | + | + | - | - | - | + | - | + | + | - | - | - | + | - | + | + |
| 3 | + | - | + | - | - | + | + | - | + | - | + | + | - | - | + | - |
| 4 | + | + | + | - | - | - | + | + | - | + | - | - | - | + | + | - |
| 5 | + | - | - | + | - | + | + | + | - | + | - | + | - | - | - | + |
| 6 | + | + | - | + | - | - | + | - | + | - | + | - | - | + | - | + |
| 7 | + | - | + | + | - | - | - | + | + | - | - | + | + | + | - | - |
| 8 | + | + | + | + | - | + | - | - | - | + | + | - | + | - | - | - |
| 9 | + | - | - | - | + | - | + | + | + | + | + | - | + | - | - | - |
| 10 | + | + | - | - | + | + | + | - | - | - | - | + | + | + | - | - |
| 11 | + | - | + | - | + | + | - | + | - | - | + | - | - | + | - | + |
| 12 | + | + | + | - | + | - | - | - | + | + | - | + | - | - | - | + |
| 13 | + | - | - | + | + | + | - | - | + | + | - | - | - | + | + | - |
| 14 | + | + | - | + | + | - | - | + | - | - | + | + | - | - | + | - |
| 15 | + | - | + | + | + | - | + | - | - | - | - | - | + | - | + | + |
| 16 | + | + | + | + | + | + | + | + | + | + | + | + | + | + | + | + |

Table V: Experimental design for 6-8 factors without confounding of individual parameters.

The results from these runs are displayed in a Pareto chart in Figure 11. It appears that the most significant factors are X2, X4, X6, and X7 along with higher order interactions between parameters, likely between these most significant factors. These factors are activation energy for reaction 1, activation for reaction 3, activation energy distribution representation for kerogen conversion, and relative permeability representation. It appears that activation energy for reaction 4 and heat of reaction have the least impact on ultimate recovery of oil.



Figure 11: Pareto chart from 16 run fractional factorial design for 8 factors.

The results from these runs can be used in a 2⁴ full factorial design without any additional runs. The data were regressed with the polynomial model and the effects are summarized in Table VI.

While the polynomial model fit the output data exactly, it is not a theoretical model and may have little physical significance. However, insight about the significance of each parameter in the explored ranges can be garnered. Typically, higher order linear interaction effects are assumed to be negligible and can be used to estimate error. Expert opinion and knowledge are also used for error estimation (Peng, 2004).

Although results for oil shale simulations in this study are calculated with theoretical governing equations, the interplay among various parameters is not trivial due to competing physical phenomena. Combinations of parameters that expose possible competing phenomena can have significant numerical implications. Molecular representations for kerogen with associated stoichiometry, heat of reaction for kerogen decomposition, intermediate oil cracking reaction (reaction 2) activation energy, and continuing gas cracking (reaction 4) reaction activation energy are insignificant in determining the ultimate recovery of oil at the scale simulated in this report. Kerogen cracking (reaction 1) activation energy, relative permeability representation, oil cracking to gas (reaction 3) activation energy, and possibly activation energy distribution representation have significant impacts on the ultimate recovery of oil in these simulations. Expert knowledge or similar studies including large scale physical experiments are important for estimating statistical error for developing validated surrogate models.

Table VI: Summary of calculated effects.

| Factors | β |
|-----------|----------|
| Intercept | 294.6071 |
| X1 | -25.9846 |
| X2 | 48.71381 |
| X3 | -8.88369 |
| X4 | -36.7407 |
| X1X2 | 17.66644 |
| X1X3 | -19.9203 |
| X1X4 | 7.082688 |
| X2X3 | 14.89081 |
| X2X4 | -2.82519 |
| X3X4 | 1.098062 |
| X1X2X3 | -5.35956 |
| X1X2X4 | 0.575937 |
| X1X3X4 | -3.37056 |
| X2X3X4 | -0.70869 |
| X1X2X3X4 | 2.191438 |

Subtask 4.3 – Multiscale Thermal Processing of Oil Shale

In this subtask, the project team is determining the weight loss and reaction kinetics of oil shale in three different sweep gas environments (nitrogen, air and carbon dioxide). The team is also performing a detailed elemental analyses of oil shale, shale oil and spent shale.

Oil shale retorting in different environments (N₂, air, CO₂)

Oil shale reaction kinetics in different gas environments may be relevant in different types of insitu processes. For example, in-situ combustion will need oil shale combustion data while pyrolysis in carbon dioxide will require kinetics of decomposition in CO₂ environments. To study these various kinetics, powdered oil shale samples were subjected to thermogravimetric analysis under these different environments. The TGA data (onset points, weight loss and temperature) are compared for pyrolysis (N₂), combustion (air) and CO₂ conditions. The data are compared at two heating rates (5°C/min and 20°C/min). The comparative TGA thermograms (Figure 12) and observed onset points (Figure 13) are shown below.



Figure 12: TGA curves for organic decomposition of oil shale in three different environments (N_2 , air, and CO_2) and at two different heating rates (5°C/min and 20°C/min).



Figure 13: TGA onset points (weight loss and temperatures) for organic decomposition of oil shale in three different environments (N₂, air, and CO₂) and at two different heating rates ($5^{\circ}C/min$ and $20^{\circ}C/min$)

The N₂ and CO₂ thermograms show only one peak while air has two peaks in the organic decomposition section. The decomposition temperature range shifts to higher temperatures as the heating rate increases for all three environments. The total organic weight loss is more in combustion (air) compared to both N₂ and CO₂. Comparatively, the temperature span with CO₂ pyrolysis is larger than with N₂, but the total organic weight losses are not significantly different.

Oil shale core sample pyrolysis - Analysis of spent shales and shale oils

Elemental analyses of oil shale, spent shale (after pyrolysis at different temperatures) and shale oils were performed using LECO CHNS-932 and VTF-900 units. The data (average of six measurements) are summarized in Table VII. The hydrogen to carbon ratio varies from about 1.2 for oil shale to 1.6 for shale oil. The spent shale hydrogen to carbon ratio varies from about 0.2 to 0.7. Most of the nitrogen ends up in the shale oil. These elemental data will help the project team validate stoichiometric models for the conversion of organic matter to oil, coke and gas.

Table VII: Elements analysis (CHNSO) of raw oil shale (OS), spent shales (SS) and shale oils (SO).

| Samples | C % | Н% | N % | S % | Ο% | Total | H/C (molar) | O/C (molar) |
|---------|-------|-------|------|------|-------|-------|-------------|-------------|
| OS_Core | 22.09 | 2.14 | 0.65 | 0.11 | 16.54 | 41.53 | 1.17 | 0.56 |
| SS_400C | 13.06 | 0.21 | 0.27 | 0.01 | 27.99 | 41.54 | 0.19 | 1.61 |
| SS_350C | 14.10 | 0.82 | 0.47 | 0.02 | 20.87 | 36.28 | 0.70 | 1.11 |
| SS_300C | 14.12 | 0.44 | 0.26 | 0.01 | 25.42 | 40.24 | 0.38 | 1.35 |
| SO_400C | 80.89 | 11.10 | 2.05 | 0.65 | 2.13 | 96.82 | 1.65 | 0.02 |
| SO_350C | 79.91 | 10.91 | 2.34 | 0.62 | 1.93 | 95.71 | 1.64 | 0.02 |
| SO 300C | 79.72 | 10.72 | 2.34 | 0.65 | 2.36 | 95.79 | 1.61 | 0.02 |

Subtask 4.4 - Effect of Oil Shale Processing on Water Compositions

In this quarter, the project team studied the effect of the presence of water on pyrolysis decomposition kinetics. Two different heating rate experiments were performed after soaking powdered shale samples in water for about five months. The soaked samples were first filtered and the TGA runs were conducted at two heating rates (5°C/min and 10°C/min). The results are compared with the TGA pyrolysis experiments at the same conditions in Figure 14.

The run at 5°C/min with the water-soaked sample shows some disturbance in the early stages of heating. This disturbance could either be instrument noise or signs of water present (free or bounded). The organic peak shifts towards higher temperatures as heating rate increases in a manner similar to that seen with "dry" pyrolysis experiments (see Figure 12). The increased weight loss observed in the experiment at 5°C/min is attributed to the variability in the organic content of the sample. The peak decomposition temperatures of water soaked samples are slightly higher than the baseline samples. The data are being analyzed to establish the kinetics of decomposition.



Figure 14: Comparison of TGA decomposition data with dry shale and samples soaked in water over a period of five months.

Subtask 4.5 - Pore Scale Analysis of Oil Shale/Sands Pyrolysis

The main thrusts of this subtask include 1) computed tomography (CT) characterization of the pore network structure for selected oil sand/oil shale resources, 2) Lattice Boltzmann (LB) simulation of flow through pore network structures to predict transport properties, such as permeability, and 3) CT analysis of pore network structure during pyrolysis reactions at different temperatures. Drill cores (1.8 cm in diameter and 5 cm in length) from a Mahogany oil shale sample and the coke products after pyrolysis were provided by Professor M. Deo from Subtask 4.3 of this research program.

The pore structure and the connectivity of the pore space are important features which determine fluid flow in oil shale during pyrolysis. In this regard, the X-ray micro/nano tomography (XMT/XNT) technique is the best non-invasive, non-destructive method available today to characterize complex pore structures. XMT/XNT captures the 3-D shape and connectivity of the void space for oil shale after pyrolysis. During this research period, the pore network structure of oil shale and the residual products after pyrolysis were further characterized with the new, high-resolution XMT (HRXMT) instrument having sub-micron voxel resolution. Figure 15 shows the 3-D volume rendered images from the reconstructed HRXMT data for the Mahogany oil shale drill core sample (MD-10). The 3-D image consists of 1024x1024x1000 voxels (volume elements) and the size of each voxel is 1.1x1.1x1.1 µm. As indicated in the left-hand side of Figure 15, lamellar structures (kerogen-rich and silicates-rich) are clearly revealed. The right-hand side of Figure 15 shows the distribution of the kerogen phase (in purple).



Figure 15. Volume rendered HRXMT images of Mahogany oil shale drill core sample MD-10 (voxel resolution = $1.1 \mu m$). Gray scale level indicates variations in the X-ray attenuation coefficients which depend on the density and atomic number of material within the voxel phase.

These results further validate previous optical microscopy results. The optical microscopy investigation of the oil shale samples confirmed the lamellar structure (Figure 16) in which different minerals are distributed in very thin and parallel laminae. These laminae include alternating layers of clay and carbonate minerals. The iron oxides and organic matter give color to the banding structure and are mostly associated with the clay mineral layers. Occasionally, they are associated with the carbonate layers. The carbonate minerals are microcrystalline. The clay mineral layers range in thickness from 0.02 to 0.03 mm in thickness, while the carbonate mineral layers range in thickness from 0.01 to 0.02 mm. The quartz mineral is of silt size and found as elongated particles parallel to the banding structure of the oil shale.



Figure 16. Micrograph showing the organic matter is mostly associated to the clay layers (MD-10 Dark Core; Plane Polarized Light).

From the image digitalization of the oil shale sample, the project team obtained the porous network structure that evolved during pyrolysis. Figure 17 shows the HRXMT images of the residual product after pyrolysis (MD-5: 5.19x5.19x8.67 mm, 400° C, N₂ flow, voxel resolution = 5.07μ m). Crack networks, developed during the pyrolysis process, are evident and can be well defined. Two distinct regions with different sizes of cracks and voids are identified and labeled "A" and "B" in the figure. Cracks and voids as small as 100 nm (from XNT images) are observed inside Region A (silicates-rich lamellar structure). In Region B, larger, anisotropic cracks and void developed (kerogen-rich lamellar structure from HRXMT images).



Figure 17. Crack networks (brown color on right-hand side) are developed inside the residual product during pyrolysis of Mahogany oil shale core sample no. 5 (MD-5: 5.19x5.19x8.67 mm, 400°C, N₂ flow, voxel resolution = 5.07 μ m). Left-hand side figure shows two distinct regions of cracks and voids, labelled "A" and "B."

As indicated in reports from a previous phase of the project, the picture obtained from XNT images of cracks and voids inside region A (silicate lamellar structure) of the oil shale pyrolysis product sample indicates that they are small and are created due to thermal expansion of grain boundaries. Figure 18 illustrates the 3-D view of the LB simulation for saturated flow through the pore space of residual products of oil shale after pyrolysis (region A). The right-hand side of Figure 18 shows the nature of the flow channels after the solid phase is removed from view. The estimated permeability from LB simulation of oil shale after pyrolysis was approximately 0.00363 μ m² or 0.363 mD.



Figure 18. 3-D views of LB simulated flow through the reconstructed XNT image of oil shale pyrolysis product sample (region A). In the left-hand side image, the white solid phase is made transparent to reveal flow channels. The right-hand side image shows the flow channels after removal of the solid phase.

In contrast, Figure 19 shows the 3-D views of LB simulated flow along the x-axis through the reconstructed HRXMT image of the oil shale pyrolysis product sample (region B). The estimated permeability in this region is 3.87x10⁻⁸ cm² or 3.92 D (darcy), which is four orders of magnitude higher than that in region A.



Figure 19. 3-D views of LB simulated flow along the x-axis through the reconstructed HRXMT image of oil shale pyrolysis product sample (region B). In the left-hand side image, the white solid phase is made transparent to reveal flow channels. The right-hand side image shows the flow channels after removal of the solid phase.

Subtask 4.6 - Kerogen/Asphaltene/Mineral Matrix: Structure and Interactions

In a previous phase of the project, the project team determined that their 12-unit kerogen model structure has a density that is comparable with experimental data (0.98 g/cm³). In this quarter, the team looked for experimental data with which to validate their model structure. Oxidation experiments performed and published in the 1960-1970 time frame suggest the presence of a high degree of cross-linking in the structure, a feature that the 12-unit kerogen model (based on the Siskin model) does not contain. Because of this deficiency, team members proceeded to modify their model to vary the degree of cross-linking in the structures. This cross-linking was done by connecting a terminal end of a molecule to an intermolecular or intramolecular double bond. Work is presently underway to determine the optimal structures using molecular mechanics minimization tools in HyperChem. Comparison with published experimental data will follow.

Preliminary results show that certain degrees of cross-linking in the structures are able to mimic published data from oxidation experiments. A second result of cross-linking one end of the molecule to a double bond is to increase the density of the model as the overall structure is more compact. This feature may allow team members to remove the artificial bounding box that is currently present in all minimization runs. Removing this restriction will enable every atom in the model to freely relax to their optimum states.

The project team also started creating entirely different models of other shale kerogens such as kukersite. The idea is to create a repository where people working in kerogen-related research activities can easily pull up the structures for comparison depending on where the sample was mined. New structures will be added to this repository once optimal structures have been determined through molecular mechanics.

Lastly, team members began looking at the stacking mechanism of asphaltene aggregates and their interaction with mineral matter. This study will enable researchers to understand how the mechanism of aggregation plays a role in residue processing and product properties.

Task 5.0 - Environmental, Legal, Economic and Policy Framework

<u>Subtask 5.1 – Land and Resource Management Issues Relevant to Deploying In-situ Thermal</u> <u>Technologies</u>

In this quarter, John Ruple, Esq., continued to monitor and review litigation challenging the federal oil shale leasing rule, the Programatic EIS for oil shale and oil sands leasing, and the multiple resource management plans containing land use stipulations applicable to oil shale and oil sands bearing lands. The outcome of this litigation is likely to impact resource access. Ruple also obtained information regarding the number, size, location, and extent of active and inactive oil sands leases on state lands within Utah in order to refine identification of areas most likely to experience development and the site-specific issues applicable to those sites. Lastly, he met with state and federal officials regarding wildlife management issues, including integrated habitat management planning and pending Endangered Species Act listing petitions that are likely to impact oil shale- and oil sands-bearing lands.

<u>Subtask 5.2 - Policy Analysis of Water Availability and Produced Water Issues Associated with</u> <u>In-situ Thermal Technologies</u>

During the fourth quarter of 2009, John Ruple, Esq., continued to monitor and review relevant litigation, rulemaking, and research relating to water resources and water quality. He obtained data from the Office of the Utah State Engineer regarding 1,661 water rights claims in the White River Basin, cleaned up and formatted the data, and began evaluating the extent and validity of

these claims. This analysis will produce a more detailed picture of existing rights, facilitating identification of those water use classifications that could be displaced by commercial oil shale or oil sands development. In order to further refine water availability assessments, Ruple confirmed management practices for the White River Basin in Colorado and Colorado's process for incorporating downstream obligations to Utah in its water availability determinations. To further refine water availability assessments, he continued research into endangered species habitat within river systems likely to provide water for commercial oil shale or oil sands development, looking specifically to instream flow recommendations contained in Biological Opinions issued by the U.S. Fish and Wildlife Service and to state policies intended to protect these flow levels. Additional water quality research focused on oil and gas process water management and water quality impacts associated with hydraulic fracturing of shallow, natural gas-bearing formations.

6.0 – Economic and Policy Assessment of Domestic Unconventional Fuels Industry

All ICSE researchers involved in the various subtasks associated with the market assessment meet on a monthly basis. This quarter, the focus of the meetings has been on selection of scenarios for the supply cost analysis as discussed in Subtask 6.3.

Subtask 6.1 Engineering Process Models for Economic Impact Analysis

For surface-mined oil shale, shale oil is produced via a retort followed by washing with hot water to remove water-soluble salts. For surface-mined tar sands, bitumen is separated from the oil via a hot water extraction process that may also remove the water-soluble salts (Netzer, 2006). The upgrading plan for the various heavy crude oils varies with the type of oil and type of upgrading methods being applied. In primary upgrading, oil that with heating can be made to flow is the desired result. A coker is used for primary upgrading for very heavy oils such as bitumen. A coker thermally cracks the long chain hydrocarbon molecules in the oil feed into shorter chain molecules and a petroleum coke residue. Secondary upgrading consists of hydrotreating the crude. Hydrotreating opens ring structures and shortens the lengths of the hydrocarbon molecules in the crude oil and also plays an important role in removing some of the sulfur as H₂S, nitrogen as ammonia and heavy metals. The hydrogen needed for hydrotreating is considerable, e.g. 350 m³ H₂ per m³ shale oil (S.G. 0.911). In this analysis, the hydrogen will be supplied by the gasification of either the heavy oil or natural gas (mostly methane). Following hydrotreating, the heavy crude oil will be of pipeline quality. The research team's approach is to determine the supply costs for the pipeline quality crude oils produced from these heavy oil deposits by these various processing routes. This analyses requires that the capital and operating costs be determined for each case.

The cases to be considered are described in Subtask 6.3. A plan has been developed for the process flow sheets needed for the various scenarios. The idea is to mix and match the needed processing steps for the three sources with the goal to meet pipeline standards for heavier oils.

Subtask 6.2 - Policy analysis of the Canadian oil sands experience

This past quarter, the project team continued research related to environmental and greenhouse gas regulatory issues and externalities associated with the Canadian experience in domestic oil sands production. Additionally, the team began research and analysis on the relevance of policy and public perception to the development of a domestic oil sands industry.

Subtask 6.3 - Market Assessment Report

Three potential sources of unconventional liquid fuels are considered for this assessment: oil shale in the Uinta/Piceance Basins, oil sands in the Uinta/Paradox Basins, heavy oil on Alaska's North Slope. Each source of unconventional liquid fuels has different chemical & physical characteristics, requiring different upstream & downstream processing operations. Figure 20 shows the basic concept of how all these processes are connected. It assumes that development objective for each resource is to produce refined products (e.g. transportation fuels, heating oil) for sale to appropriate markets. Each box in the figure will require specific information depending on the resource being considered.



Figure 20. Overview of processing operations required for production of unconventional liquid fuels.

In this quarter, the goal was to create a wide range of possible configurations and then establish criteria for filtering this range of scenarios to a manageable list of 5-6 scenarios (1-3 configurations for each of the three region-resource areas). The goal is to choose scenarios that produce the lowest supply cost for a range of plausible states of the world. These scenarios should also span the range of preparedness for non-free CO₂. Possible criteria/assessment tools for this filtering step include:

- Externalized public costs
- Data availability
- Likelihood of industrial cooperation
- Potential cost of CO₂ emissions/CO₂ footprint
- Cost/availability/usage of water

- Cost/availability of natural gas
- Cost of various environmental remediation/mitigation (e.g. reclamation)
- Likely market for refinery outputs
- Observing and noting what firms are already doing
- Quality of reservoir (barrels per acre)
- Cost/availability/usage of external power sources

After a series of meetings to discuss possible criteria for refining the scenarios, the project team decided on the following list:

1. Data availability and likelihood of industrial cooperation - Reliable supply costs are dependent on industrial-scale data and accurate models where data are not available. Those models in turn require some type of data, although not necessarily at an industrial scale. The project team is in discussions with both heavy oil and oil sands companies to use their data in the supply cost analysis. Additional data from pilot- or demonstration-scale facilities will be used for scale up.

2. Environmental impacts, particularly the CO₂ footprint and possibility of CO₂ mitigation and the water requirements - Given the current political climate, the likelihood of establishing a CO₂-intensive industry seems unlikely. In fact, a coalition of 142 shareholders of Royal Dutch Shell have asked the company for a review of the risks associated with their Canadian oil sands projects given the likely increase in carbon costs (Pals, 2010). In addition, water is a scarce resource in the arid West where the major U.S. oil shale and oil sands deposits are located. Scenarios must account for these two pressing environmental concerns.

Work also continued this quarter on the revenue side of the viability issue. ICSE economist Michael Hogue is using time-series multiple regression techniques to isolate the effects on the product price (relative to the price of a marker crude---so this is a "differential") which can be attributed to certain physical properties of the crude (e.g. API, sulfur and nitrogen content, TAN).

CONCLUSIONS

The Clean and Secure Energy from Domestic Oil Shale and Oil Sands Resources program enhanced its outreach to industry and increased collaborations within ICSE via various field trips, presentations, and seminars. Research work focused on four main areas. In the area of oil shale and sands utilization with CO₂ management, the groundwork was laid for future efforts at estimating the potential for CO₂ emissions reductions in upgrading and refining facilities via oxygas combustion and at developing a simulation tool for use in oxy-gas process heaters. In the area of liquid fuel production from in-situ thermal treatment of oil shale/sands, the research team focused on vertical integration via a standard sample and on developing models (e.g. permeability, pyrolysis kinetics) that can be used in an integrated in-situ simulation. In the area of environmental and policy frameworks, ongoing litigation and rulemaking related to land use impacts and water quality/quantity impacts of in-situ oil shale/sands development was monitored for future analysis and reporting. In the market assessment area, the project team established criteria for selecting unconventional fuel production scenarios on which to perform a supply cost analysis and began work to determine which physical properties of crude affect the product price in consideration of the revenue side of the viability equation.

COST STATUS

| | Yr. 1 | | | | | | | | | |
|----------------------------|-------------|---------|----------|-----------|---------|-----------|----------|-----------|--|--|
| Descling Departing Quarter | Q1 | | U U | Q2 | | 23 | Q4 | | | |
| Daseline Reporting Quarter | 7/1/09 - 12 | 2/31/09 | 1/1/10 - | 3/31/10 | 4/1/10 | - 6/30/10 | 7/1/10 - | 9/30/10 | | |
| | Q5 | Total | Q6 | Total | Q7 | Total | Q8 | Total | | |
| Baseline Cost Plan | | | | | | | | | | |
| Federal Share | 484,728 | 484,728 | 484,728 | 969,456 | 484,728 | 1,454,184 | 484,726 | 1,938,910 | | |
| Non-Federal Share | 121,252 | 121,252 | 121,252 | 242,504 | 121,252 | 363,756 | 121,254 | 485,010 | | |
| Total Planned | 605,980 | 605,980 | 605,980 | 1,211,960 | 605,980 | 1,817,940 | 605,980 | 2,423,920 | | |
| Actual Incurred Cost | | | | | | | | | | |
| Federal Share | 420,153 | 420,153 | | 420,153 | | 420,153 | | 420,153 | | |
| Non-Federal Share | 29,456 | 29,456 | | 29,456 | | 29,456 | | 29,456 | | |
| Total Incurred Costs | 449,609 | 449,609 | 0 | 449,609 | 0 | 449,609 | 0 | 449,609 | | |
| Variance | | | | | | | | | | |
| Federal Share | 64,575 | 64,575 | 0 | 549,303 | 0 | 1,034,031 | 0 | 1,518,757 | | |
| Non-Federal Share | 91,796 | 91,796 | 0 | 213,048 | 0 | 334,300 | 0 | 455,554 | | |
| Total Variance | 156,371 | 156,371 | 0 | 762,351 | 0 | 1,368,331 | 0 | 1,974,311 | | |

| | Yr. 2 | | | | | | |
|----------------------------|-------------|-----------|----------|-----------|--|--|--|
| Receive Reporting Quarter | Q5 | | Q6 | | | | |
| Baseline Reporting Quarter | 10/1/10 - 1 | 2/31/10 | 1/1/11 - | 3/31/11 | | | |
| | Q8 | Total | Q8 | Total | | | |
| Baseline Cost Plan | | | | | | | |
| Federal Share | 323,403 | 2,262,313 | 323,402 | 2,585,715 | | | |
| Non-Federal Share | 80,835 | 565,845 | 80,834 | 646,679 | | | |
| Total Planned | 404,238 | 2,828,158 | 404,236 | 3,232,394 | | | |
| Actual Incurred Cost | | | | | | | |
| Federal Share | | 420,153 | | 420,153 | | | |
| Non-Federal Share | | 29,456 | | 29,456 | | | |
| Total Incurred Costs | 0 | 449,609 | 0 | 449,609 | | | |
| Variance | | | | | | | |
| Federal Share | 0 | 1,842,160 | 0 | 2,165,562 | | | |
| Non-Federal Share | 0 | 536,389 | 0 | 617,223 | | | |
| Total Variance | 0 | 2,378,549 | 0 | 2,782,785 | | | |

Baseline Cost Plan is based on the proposal's budget pages (SF424a)
Q1 includes pre-award, incurred and pending postings (\$47,152). Matching costs that are at a low percent of total will adjust to the required percentage over the quarters to follow.

MILESTONE STATUS

Subtask 6.3, the market assessment report, had a milestone scheduled for completion in this quarter. The milestone, to identify and describe criteria used to select scenarios, was reported in the Subtask 6.3 summary above.

PROBLEMS OR DELAYS

For Subtask 4.5, the work has been impeded by the availability of nano CT to characterize the oil shale samples at nano scale.

RECENT AND UPCOMING PRESENTATIONS/PUBLICATIONS

Jake Bauman and Milind Deo, "Interaction Between Reactivity and Flow in the In-situ Production of Oil from Oil Shale." Presentation at the 29th Oil Shale Symposium, Colorado School of Mines, Golden, CO, October 19-23, 2009.

Michelle Kline, Wendy Ajax, Kirsten Uchitel, and Jennifer Spinti, "The Digital Library and Interactive Map Projects at the Institute for Clean and Secure ENergy, University of Utah." Poster presented at the 29th Oil Shale Symposium, Colorado School of Mines, Golden, CO, October 19-23, 2009.

Chen Lu Lin, Jan Miller, C. H. Hsieh, Pankaj Tiwari and Milind Deo, "Pore-scale Analysis of Pyrolyzed Oil Shale Cores." Presentation at the 29th Oil Shale Symposium, Colorado School of Mines, Golden, CO, October 19-23, 2009.

Pankaj Tiwari and Milind Deo, "Oil Shale Pyrolysis: Characterization and Compositional Analysis." Poster presented at the 29th Oil Shale Symposium, Colorado School of Mines, Golden, CO, October 19-23, 2009.

Pankaj Tiwari and Milind Deo, "Kinetics of Oil Shale Pyrolysis and Composition of the Produced Shale Oil" in *Oil Shale: Solutions to the Liquid Fuel Dilemma*, ACS, in press.

Chung-kan Huang, Jake Bauman, and Milind Deo, "Modeling of the In-situ Production of Oil from Oil Shale" in *Oil Shale: Solutions to the Liquid Fuel Dilemma*, ACS, in press.

Kirsten Uchitel, Robert Keiter, and John Ruple, "Environmental and Policy Issues Relevant to Oil Shale Development Under the Energy Policy Act of 2005" in *Oil Shale: Solutions to the Liquid Fuel Dilemma*, ACS, in press.

John Ruple and Robert Keiter, "Water for Commercial Oil Shale Development in Utah: Allocating Scarce Resources and the Search for New Sources of Supply" in *Journal of Land, Resources & Environmental Law*, in press.

John Ruple and Robert Keiter, "Water for Commercial Oil Shale Development in Utah: Clarifying How Much Water is Needed and Available," International Bar Association, *Journal of Energy & Natural Resources Law*, in press.

C.H. Hsieh, C.L.Lin and J.D. Miller, "Pore Scale Analysis of Oil Sand/Oil Shale Pyrolysis by Xray Micro CT and LB Simulation." To be presented at Student Poster Section, SME Annual Meeting, February 28 – March 3,2010, Phoenix, AZ. I.S.O. Pimienta, A.M. Orendt, R.J. Pugmire, and J.C. Facelli, D. R. Locke, R. E. Winans, K. W. Chapman, and P. J. Chupas, "Three-Dimensional Structure of the Siskin Green River Oil Shale Kerogen Model: A Computational Study." Manuscript has been written for submission to the journal *Energy Fuels* pending approval from funding sources.

Steve Burian, "Relative Influence of Hydrologic Cycle Changes Caused by Climate Variability on the Feasibility of White River Streamflow and Reservoir Capacity to Meet Energy Demand Requirements," to be submitted to a journal in March 2010.

Lauren P. Birgenheier and Michael D. Vanden Berg, "Integrated Sedimentary and Geochemical Investigation of Core From the Upper Green River Formation Lacustrine Deposits, Uinta Basin, Utah." Poster to be presented at the 2010 AAPG Annual Meeting, New Orleans, LA, April 12, 2010.

C.L. Lin, A.R. Videla and J.D. Miller, "Advanced 3D Multiphase Flow Simulation in Porous Media Reconstructed from X-ray Micro Tomography Using the He-Chen-Zhang Lattice Boltzmann Model." Manuscript submitted to *Flow Measurement and Instrumentation*.

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