

Oil & Natural Gas Technology

DOE Award No.: DE-FE0001243

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

Quarterly Progress Report (January – March 2010)

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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EXECUTIVE SUMMARY

The Clean and Secure Energy from Domestic Oil Shale and Oil Sands Resources program is part of the research agenda of the Institute for Clean and Secure Energy (ICSE) at the University of Utah. In this quarter, the Clean and Secure Energy program continued its focus on enhancing industrial, national laboratory, and academic connections with visits from Calera, Praxair, Sage Geotech, Sandia National Lab, Idaho National Lab, and Los Alamos National Lab and a visit to Utah State University to discuss opportunities for intrastate collaboration on energy-related projects. Efforts to enhance ICSE outreach tools (the repository, the interactive map, and the website) also continued. The current focus of the repository is to upload publications by ICSE researchers. The interactive map has been augmented with water-related data. Two new features were also added to the interactive map: the ability to save the map as an image (and print it, if desired), and the ability to search for features on the map by name. A new ICSE website was rolled out in January that is meant to better reflect the multidisciplinary nature of ICSE and to provide easier access to ICSE information and outreach tools.

In Task 3.0, ICSE researchers have finished gathering literature data on the potential of oxy-fuel for CO₂ capture in refining and oil sands upgrading operations and have computed estimates of life-cycle well-to-pump CO₂ emissions for crude oil refining under both baseline and process heater oxy-firing conditions. Researchers are also performing simulations of the oxy-gas fired test furnace at the International Flame Research Foundation. The initial test matrix considers two scenario parameters (natural gas and O₂ flow rates) and one model parameter (boundary condition applied to the walls of the computational domain). Each simulation requires 360 processors for approximately 72 hours. The simulations are currently being run on ICSE computing facilities.

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 in-situ thermal treatment of oil shale/sands. Discussion this quarter focused on obtaining a fresh core sample from the Mahogany zone of the Green River Formation in Utah's Uinta Basin. A plan to piggyback on drilling that Oil Shale Exploration Company (OSEC) will be conducting this spring on their private land has been made. The Subtask 4.1 team determined that the simulation of the ECOSHALE capsule needed to include the actual geometry of the pieces of shale. The simulation software Star-CCM+ can handle a complex geometry and can accurately model the convective currents through the channels of the rubble bed found within the ECOSHALE capsule. The Subtask 4.2 team constructed the west-to-east (W-E) cross section of 4 wells across a 24-mile region in Utah's Uinta Basin with a goal to provide better geologic models to reservoir simulations in the basin. The team also studied the application of the Friedman method and "model free" methods to better determine the relationship between conversion and activation energy in kerogen conversion kinetics for reservoir simulation. Researchers in Subtask 4.3 used thermo-gravimetric analysis (TGA) with mass spectrometry (MS) to study pyrolysis of oil shale samples at different heating rates. The addition of MS to the TGA experiments allows for product identification as the pyrolysis process unfolds. The Subtask 4.4 team collected oil and water samples from hydrous pyrolysis experiments to compare with the non-hydrous (ordinary) pyrolysis. Aromatics and alkenes were higher in concentration in hydrous pyrolysis compared to ordinary pyrolysis at the same conditions. The water samples will be sent to a commercial laboratory to obtain concentrations of dissolved organics. In Subtask 4.5, the team performed detailed 3D imaging of oil shale core before and after pyrolysis. The pore structure of the pyrolyzed samples deduced from the images was used for Lattice Boltzmann simulations to calculate the permeability in the pore space. The permeabilities of the silicate-rich zone were on the order of milli-Darcies, while the reacted core permeabilities of the kerogen-rich zone were very anisotropic and about four orders of magnitude higher. ICSE researchers in Subtask 4.6 began ab initio calculations and molecular

dynamics simulation of asphaltenes with the objectives of developing 3D models of asphaltenes based on existing 2D model, studying agglomeration of asphaltenes and studying the interaction between asphaltenes and mineral matter.

In Task 5.0, ICSE researchers continued to monitor and review litigation challenging the federal oil shale leasing rule, the Programmatic 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. Researchers also completed and submitted a Topical Report entitled "Policy Analysis of Water Availability and Use Issues For Domestic Oil Shale and Oil Sands Development."

In Task 6.0, the research team developed a methodology to be used for the economic analysis of various heavy oil production methods and subsequent upgrading methods. Supply costs for the various scenarios will use industrial standard methods for the estimation of capital and operating costs for each year over the life of the project and standard accounting methods to establish discounted cash flow predictions for the project. The team also reviewed and began drafting analysis of research related to the realities and perceptions of the carbon footprint of oil sands development in Canada. Lastly, researchers identified and described the methodology applied to assess the impact of downstream market conditions on potential revenue from upstream scenarios. Oil price risk will be accounted for using a model of the price of the West Texas Intermediate (WTI) marker crude with parameters of this model established from oil price data and also tuned to reflect "what if" scenarios for the level and volatility of the future prices of oil.

PROGRESS, RESULTS, AND DISCUSSION

Task 1.0 - Project Management and Planning

The project management plan (PMP) was approved by NETL in the previous quarter. There were no schedule/cost variances or other situations requiring updating/amending of the PMP in this quarter.

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. As part of this task, ICSE organized and held the Energy Forum event at the University of Utah law school on February 3, 2010. The Energy Forum included representatives from industry, academia and government who participated in a moderate panel discussion of the role of unconventional fossil fuels in the nation's energy portfolio and the environmental challenges associated with these fuels. The Forum was open to the public and drew approximately three hundred attendees. Work also occurred during this quarter on organizing the University of Utah Unconventional Fuels Conference and the ICSE Industrial Advisory Board Meeting, both scheduled for April 2010. ICSE continued to develop its relationship with industry and policymakers through visits and/or roundtables with Randy Seeker from Calera, representatives from Idaho National Laboratory, representatives from the Government Accountability Office, Sho Kobayashi from Praxair, Gary Aho, from Sage Geotech, and Jim Nakos from Sandia National Laboratory. ICSE also participated in USTAR's Uintah Basin Black Wax Workshop.

Other major outreach activities during this quarter include the continued expansion of the ICSE repository and interactive map. The Institute Librarian, Wendy Ajax, is working with

administrators of the private DSpace collections, reviewing and culling these collections for documents that can be added to the public DSpace community. Work also continues on gathering and uploading publications of ICSE researchers. Full text versions of scholarship generated by ICSE researchers are being uploaded to the ICSE private community and, where copyright permission can be obtained, the public community. When copyright permission cannot be obtained, abstracts are being uploaded to the public community.

For the ICSE interactive map project, GIS Applications Developer, Michelle Kline, focused on incorporating the water management geodatabase into the map. The following water management datasets were included with the geodatabase and have been added as layers to the map: water quality assessment units, wetlands, hydrologic units, dams, watersheds, water-related land use, water rights, adjudication areas, and shallow groundwater aquifers. These new map layers lie within the state of Utah. In addition, a national dataset reflecting U.S. EPA 303(d) Listed Impaired Waters was obtained and added to the interactive map as a layer. With these new datasets, a user of the interactive map might select some features in the Utah water quality assessment units layer, view the description and protected status of each unit, and search for documents in the digital repository which reference the unit names.

Additional improvements were made to the map based on feedback from beta version map testers. These improvements include refining the attribute data associated with features in the oil shale map layers, relaxing the restrictions that prevent map users from viewing features at all scales, and replacing the outdated "Utah Current Tar Sands Resources" layer with the newer "North American Oil Sands Resources" layer. Two new features were also added to the interactive map: the ability to save the map as an image (and print it, if desired), and the ability to search for features on the map by name.

Work to be conducted on the interactive map during the second quarter of 2010 will be focused on implementing a method for tracking and analyzing interactive map usage. Testing of website tracking software has already begun and will be fully implemented during the upcoming quarter.

The ICSE Web Applications Programmer, Terrance Davis, completed the testing, debugging, and migration of the Dspace source for use with the new PostgreSQL database. He also installed and configured a new database server for use with Dspace and with the ICSE content management system. Work began on documenting the ICSE repository code and database using UML. Lastly, the new, more integrated ICSE website was deployed during this quarter. The new website has improved links to research projects, the ICSE repository and interactive map, and a 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 focused their data gathering on the potential of oxy-fuel combustion for CO₂ capture in refining operations. They have also been coordinating with investigators from the other subtasks to gather data on oil sands upgrading. Because more information is available for refining operations than for upgrading, the initial analysis is based on a study by Allam et al. (2005) for the British Petroleum Grangemouth refinery in Scotland. In the study, they estimated the costs and CO₂ emissions from converting seven boilers and process heaters to oxy-firing for CO₂ capture. Their estimates included building and operating an air-separation unit (ASU) and a gas turbine (NGCC) to provide power for the ASU plus the necessary CO₂ purification, compression, and delivery to fenceline costs. They evaluated the following three cases:

- Case 1: A gas turbine and associated steam production provides power for the ASU and CO₂ purification, compression, etc.
- Case 2: A gas turbine provides power to the ASU and other equipment, but steam from the turbine replaces a portion of the boiler steam. This results in a lower O₂ requirement, a smaller ASU, and less cooling water.
- Case 3: The gas turbine is run in the precombustion decarbonisation mode with part of the O₂ being used for hydrogen production and CO₂ removal using MDEA.

To these estimates, team members added the upstream life-cycle CO₂ emissions for conventional oil production using Argonne National Laboratory's GREET model. These upstream emissions included the additional CO₂ emissions associated with the extraction and transport of the additional natural gas required to power the gas turbine engine. The results, shown in Figure 1, include the efficiency evaluation discussed in the previous quarterly report. CO₂ emissions associated with the additional natural gas are shown in bright green for the refining stage and medium blue for the extraction and transportation stages.

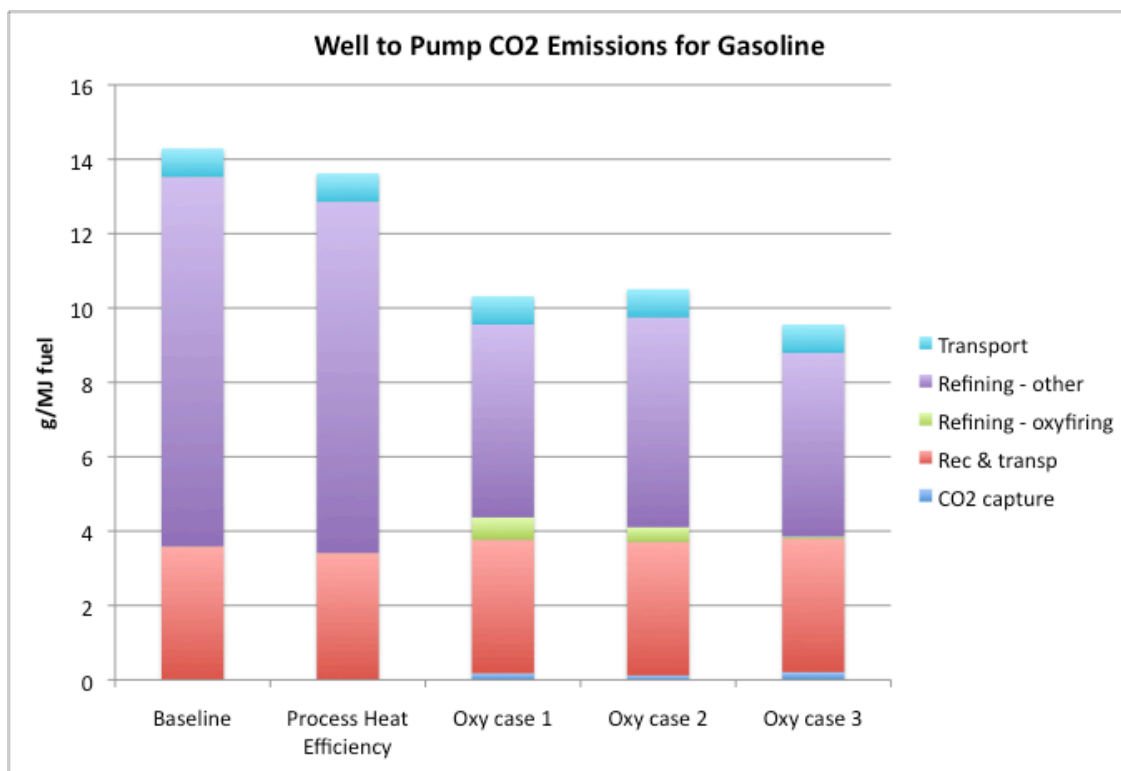


Figure 1. Comparison of well-to-pump CO₂ emissions for gasoline production from an average refinery (baseline) and from a refinery using oxy-firing to capture approximately 40% of the CO₂ emissions for three different cases (described above).

Allam's study found that approximately 40% of their refinery's CO₂ could reasonably be captured from relatively concentrated sources of CO₂ such as boilers and process heaters, at a cost ranging from \$34 -38/tonne CO₂ captured. Once the additional emissions from the gas turbine and upstream CO₂ emissions are considered, this results in approximately 28 – 34% of the CO₂ being avoided (Table 1). The project team is now in the process of including other greenhouse gases (i.e., CH₄ and N₂O) in the analysis.

Table 1. Summary of well-to-wheel life-cycle CO₂ emissions and carbon-capture costs (g/MJ gasoline).

Refinery	Energy recovery & transport	Excess recovery & transport	Refining		CO ₂ (only) Total	% Reduction	Cost \$/CO ₂ tonne*
			Refining Oxy	Refining Other			
Baseline	3.59	0		9.94	0.451	14.0	0
Improved efficiency	3.41	0		9.45	0.451	13.3	4.9
Oxy case 1	3.59	0.177	0.604	5.26	0.451	9.97	29
Oxy case 2	3.59	0.119	0.401	5.74	0.451	10.2	28
Oxy case 3	3.59	0.208	0.0545	4.15	0.451	8.50	34

*CO₂ captured/avoided

** Improved process heater efficiency (100 mmBTU/hr) requires increased capital costs, 1.5* conventional (\$8.1M/\$5.2M) but results in fuel savings of \$92K/yr, making it cost effective with a 15 yr recovery period and a 12%IR.

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

As noted last quarter, the project team has selected the International Flame Research Foundation's (IFRF) OXYFLAM experiments as the foundation for their verification/uncertainty quantification analysis. These oxy-gas datasets were collected in 1995-1996 in the IFRF Furnace No. 2 (Lallement et al., 1997) as shown in Figure 2. The furnace has a total length of 3.9 m and a cross section of 1.2 m x 1.2 m. After evaluating the IFRF case further, the project team decided to focus computational resources on the near-burner region of the furnace. The computational domain is 1.23 m in length with a 0.735 m x 0.735 m cross section. The observed flame diameter in the OXYFLAM-1 experiments was 10-20 cm near the burner and 50-60 cm at an axial distance of 1 m downstream of the burner, so the computational domain is sufficient to capture flame spread in the near-burner region. The computational mesh is 275 x 190 x 190, resulting in 4.5 cm resolution in the length direction and 3.9 cm resolution in the cross-section directions.

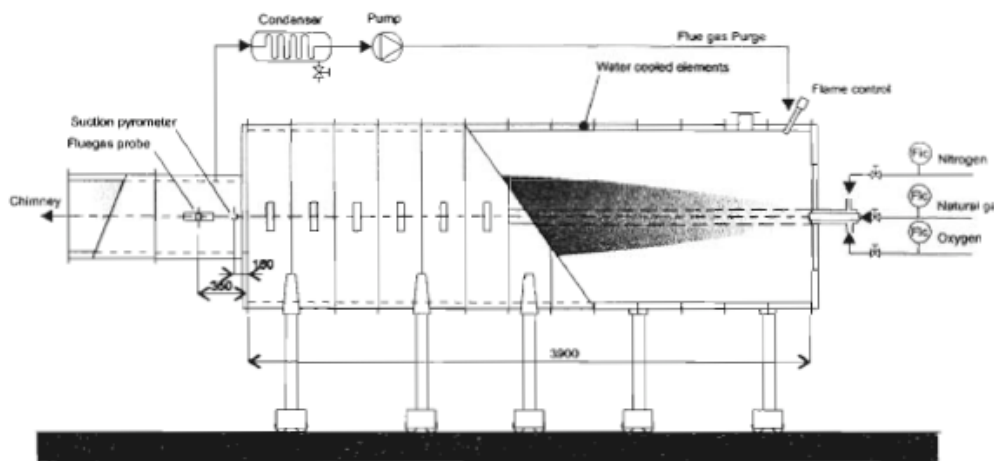


Figure 2: Configuration of IFRF Furnace No. 2 for OXYFLAM experiments (Lallement et al., 1997).

In the OXFLAM tests, two wall conditions and three different burners were evaluated (Lallement et al., 1997). For this initial phase of the project, the chosen boundary conditions most closely match those observed in the OXFLAM-2 experiments, which were conducted in a refractory-lined furnace. The three oxy-natural gas burners were based on the same generic, double pipe design. The variable in the burner design was the diameter of the pipes, leading to high, medium, and low momentum burners. The project team selected the low-momentum burner, Burner C, for the work reported here.

A face-centered composite (FCC) experimental design is being used for the simulations. The FCC design typically involves 3 evenly-spaced levels (low, medium, and high) of each parameter. The parameters chosen for the first phase of this analysis are two scenario parameters and one model parameter. The scenario parameters are the natural gas flow rate and the O₂ flow rate. The model parameter is the boundary condition applied to the walls of the computational domain. After reviewing variability in measured flow rates and estimated instrument uncertainties for both natural gas and O₂, the error in the natural gas flow rate was estimated to be +/-5% and the error in the O₂ flow rate was estimated to be +/-3%. The boundary condition applied at the walls of the domain was varied to reflect different levels of heat loss based on a fully-mixed, fully-reacted system. The skeletal design matrix (no mid-points included) consisting of 8 cases that span this parameter space is listed in Table 2. In this table, a value of 0 in the boundary heat loss column refers to an adiabatic condition as the boundary model while a value of 1 refers to maximum theoretical heat loss at a fully-mixed, fully-reacted condition.

Table 2. Summary of FCC three-parameter skeletal design matrix for the IFRF OXYFLAM-2 tests with Burner C.

Case No.	O ₂ inlet, kg/s	Natural gas inlet, kg/s	Boundary heat loss	Box location
1	1.663E-02	6.049E-02	0	low, low, low
2	1.838E-02	6.049E-02	0	high, low, low
3	1.663E-02	6.423E-02	0	low, high, low
4	1.663E-02	6.049E-02	1	low, low, high
5	1.838E-02	6.423E-02	0	high, high, low
6	1.663E-02	6.423E-02	1	low, high, high
7	1.838E-02	6.049E-02	1	high, low, high
8	1.838E-02	6.423E-02	1	high, high, high

The eight simulations listed in Table 1 are currently being run on ICSE computing resources. Each case requires 360 processors for approximately 72 hours. Figure 3 shows the vorticity field for Case 1. The case is still being run to generate enough output timesteps for statistically-stationary time-averaging. Once the simulations are all completed, a Data Collaboration analysis will be initiated.

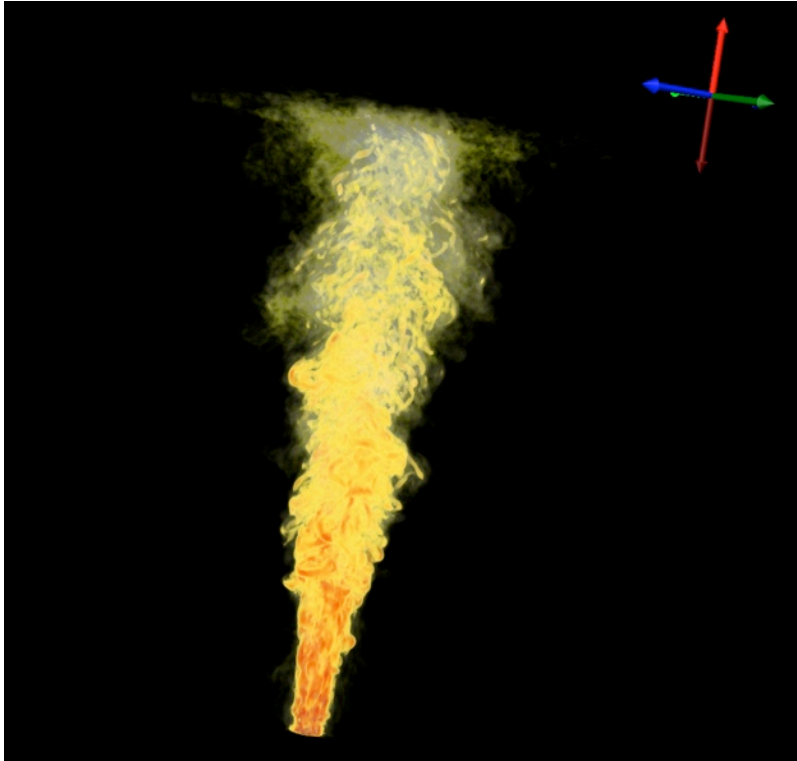


Figure 3: Vorticity field for IFRF Burner C in OXYFLAM-2 experiment.

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

In meetings of Task 4.0 researchers this quarter, discussion focused on obtaining a fresh core sample from the Mahogany zone of the Green River Formation in Utah's Uinta Basin. A path forward was identified with the help of Gary Aho from Sage Geotech. The plan is to piggyback on drilling that Oil Shale Exploration Company (OSEC) will be conducting this spring on their private land. OSEC has agreed in principle to allow the University of Utah to drill on their land and use the core obtained for research purposes.

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

In order to perform a validation/uncertainty quantification analysis of the Red Leaf ECOSHALE test capsule, the project team initially envisioned creating a simulation tool with ARCHES that would use a statistical approach to model the geometry, e.g. voids and physical pieces of shale. However, researchers determined that a better simulation tool for this process was one which included the actual geometry of the pieces of shale. Performing this type of simulation in ARCHES is difficult due to the complex geometry. The simulation software Star-CCM+ is capable of producing a simulation tool that can handle a complex geometry and can accurately model the convective currents through the channels of the rubble bed found within the ECOSHALE capsule. Scaling studies performed on Star-CCM+ for other cases performed at ICSE suggest that Star-CCM+ will be able to scale for the large computational size of the problem.

During this quarter, the project work has included the creation of a complex shale geometry and initial simulation preparations in Star-CCM+. DEM Solutions product EDEM, a discrete element modeling software used for modeling particle movement, was used to simulate the filling of an empty bed with pieces of oil shale. This simulation models the interactions between particles and geometry as they fall into the bed. The simulation resulted in a bed full of thousands of pieces of oil shale that can be used as a representation of the actual rubblized bed. The EDEM simulation provided data for position, size, and rotation of each particle.

Matlab was used to write a journal file that defines the particles as they lay in the EDEM simulation. The journal file was run in the CAD software Gambit, and the shale geometry was created. Figure 3 shows a representation of the shale geometry in Gambit.

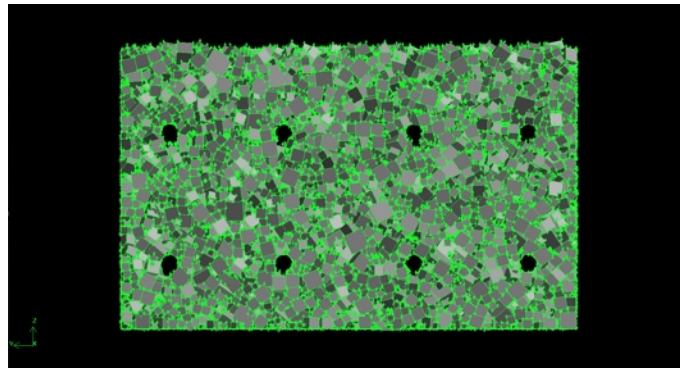


Figure 4. Image of shale geometry created in Gambit.

Gambit produces a parasolid transmit file, a standard geometry file type that can be used in Star-CCM+. Implementation of the correct geometry representation in Star-CCM+ requires additional work in creating boundary interfaces between pieces of shale and fluid.

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

For the basin-wide characterization portion of the subtask, the project team described the P-4 core and completed its geochemical analysis. Team members also constructed the west-to-east (W-E) cross section of 4 wells across a 24-mile region. Figure 5 indicates the geographic location of the W-E cross section while Figure 6 shows its constructed cross section.

For the second part of the subtask involving in situ production models, previous work has found that representation of kinetic parameters within reasonable ranges can have significant impact on the ultimate recovery of oil from oil shale resources predicted by the simulation. Specifically, average kerogen cracking activation energy and the kerogen cracking activation energy distribution representation were highlighted as two significant parameters. The appropriate kinetic model for kerogen conversion is unclear. The Arrhenius model is shown in Equation 1. The rate is calculated with some kinetic model, $f(\alpha)$, where, in this case, α is conversion.

$$k = A \cdot e^{-\frac{E_{act}}{R_g \cdot T}} \quad (1)$$

$$R = \frac{d\alpha}{dt} = k \cdot f(\alpha) \quad (2)$$

In chemical kinetic studies, experiments are typically run with varied time and temperature histories to give rate data where constant parameters A and E_{act} are calculated. The ability to calculate these constant parameters based on the experimental data depends on the reality of the assumed $f(\alpha)$. Depending on the experimental conditions, $f(\alpha)$, A , and E_{act} can be molded to fit the experimental data. In well designed experiments, these three parameters can be interpolated and extrapolated to accurately predict different time and temperature conditions. Unfortunately, for some complex processes, including kerogen pyrolysis, the solutions for $f(\alpha)$, A , and E_{act} are not necessarily unique, and one set of parameters that fits a set of experimental data may be unable to predict the behavior of another experiment and may be completely infeasible when extrapolated to large scale systems.

One common method for resolving this dilemma is the Friedman method. The Friedman method assumes $f(\alpha)=1-\alpha$ and finds parameters A and E_{act} for each specific conversion. Parameters A and E_{act} are therefore dependent on conversion. Another way researchers have dealt with similar problems is with “model free” methods. These methods combine parameters A and $f(\alpha)$ and allow a relationship between conversion and E_{act} , referred to as a distribution of activation energies. The following rate equation is the result. Parameters $Af(\alpha)$ and $E_{act}(\alpha)$ are calculated for each value of

$$\frac{d\alpha}{dt} = Af(\alpha) \cdot e^{-\frac{E_{act}(\alpha)}{R_g \cdot T}} \quad (3)$$

conversion, leading to distributions for $Af(\alpha)$ and $E_{act}(\alpha)$. $Af(\alpha)$ and $E_{act}(\alpha)$ were found with IsoKin software. Figure 7 shows the fit of a polynomial model used to estimate $\ln(Af(\alpha))$. A similar polynomial fit was used to estimate $\ln(E_{act}(\alpha))$.

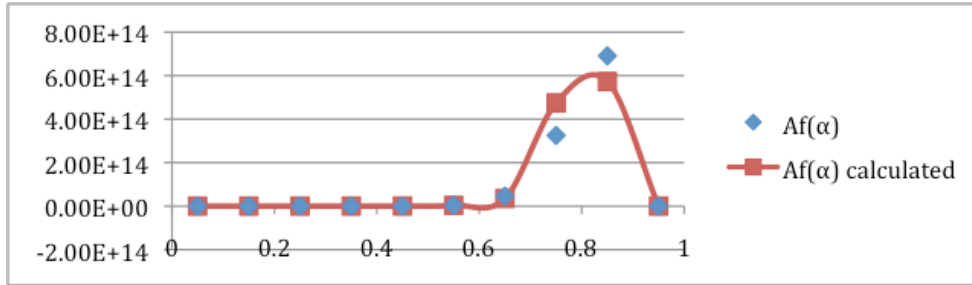


Figure 7: Regression model used to estimate $Af(\alpha)$.

Polymath 5.1 software was used to solve this reaction rate ODE with a 10°C/min heating rate. The Polymath plots shown in Figure 8 compare the solutions of equations (3) and (2) where $f(\alpha) = (1-\alpha)$ with a variety of potential constant parameters A and E_{act} . These parameter values were calculated using the IsoKin solution data, which was obtained using the experimental TGA data. Table 3 lists the parameter values used to obtain the plots in Figure 8.

Table 3: Actual values of kinetic parameters used to obtain Polymath plots.

	E (kJ/mol)	A (first order)
average	180.3468645	6.46275E+16
median	189.3079226	3.2138E+13
min	88.072	629917.7676
max	249.6162696	7.12149E+17

It should be noted that although certain pairs of parameters A and E are vastly different, they do not necessarily have extremely different solutions for rate. Alternatively, when the combination of average A and E values are used, the rate is extremely fast in comparison to all other results. This can lead one to infer the major interplay between parameters A , E_{act} , and $f(\alpha)$. The experimental conditions and methods for analysis to determine these parameters have significant impact on the reaction rate.

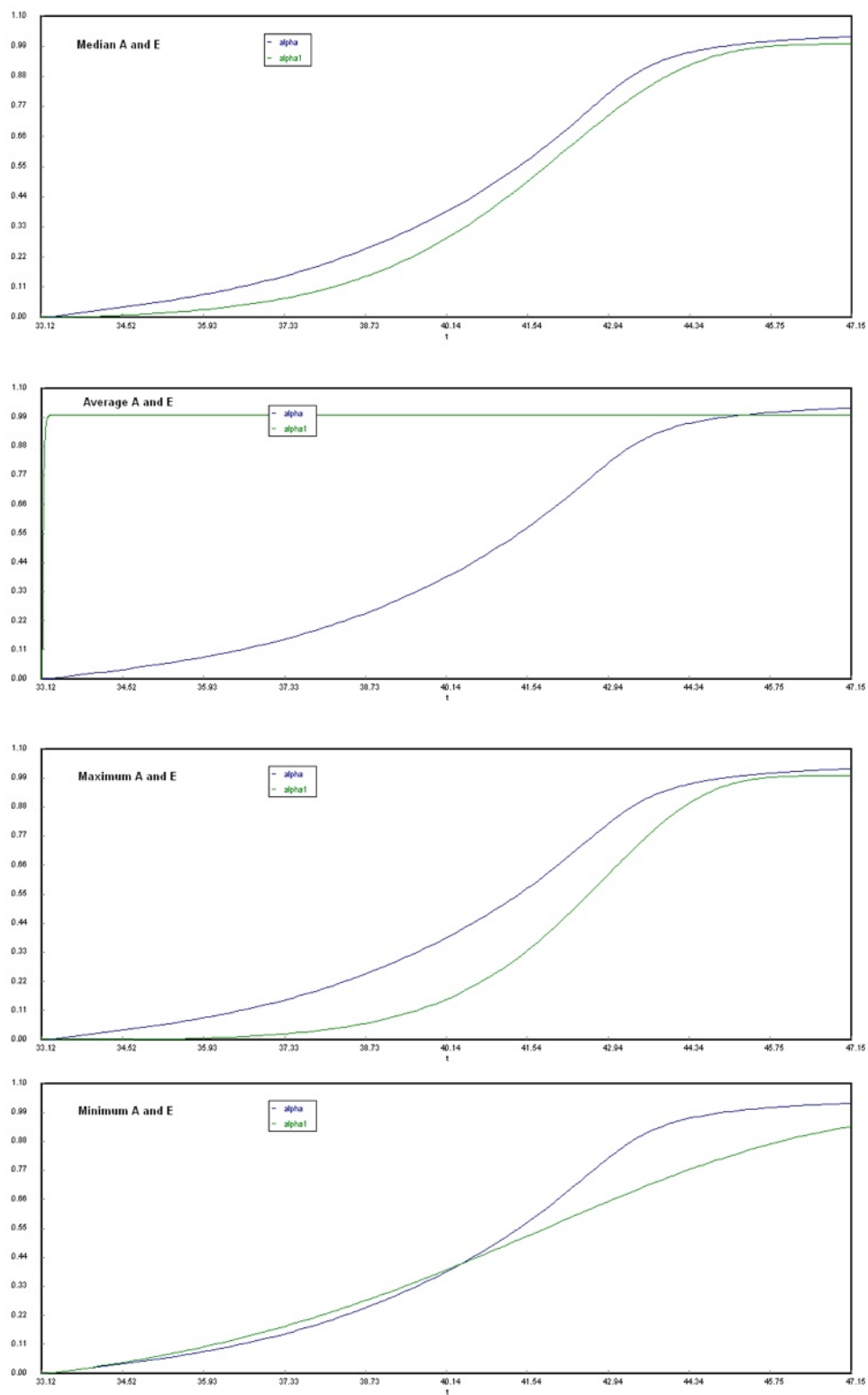


Figure 8: Polymath plots of conversion vs. time for various combinations of kinetic parameters.

Subtask 4.3 – Multiscale Thermal Processing of Oil Shale

In this subtask, the project team used thermo-gravimetric analysis (TGA) with mass spectrometry (MS) to study pyrolysis of oil shale samples at different heating rates. The mass spectrometer is used to identify the products of reactions. The experimental conditions and information obtained from the TGA weight loss curve are summarized in Table 4. The experiment at 5°C/min was repeated to ensure the reproducibility of results. The TGA thermograms are depicted in Figure 9. The weight loss curves were almost identical those generated in previous experiments with the TGA alone.

Table 4: TGA-MS experimental conditions and weigh loss data.

Heating rate	Final temperature	Total compounds	Weight, mg	%wt loss @250C	%wt loss @500C	%wt loss @600C	T _{max} , C
0.5C/min	650C	43	22.54	0.34	9.38	20.14	401.03
1C/min	600C	56	13.10	0.65	9.6	15.99	413.09
5C/min-1	960C	22	13.34	0.59	10.76	13.2	442.61
5C/min-2	600C	56	13.26	0.46	10.3	11.29	443.41
10C/min	650C	41	19.05	0.63	11.28	12.47	456.93

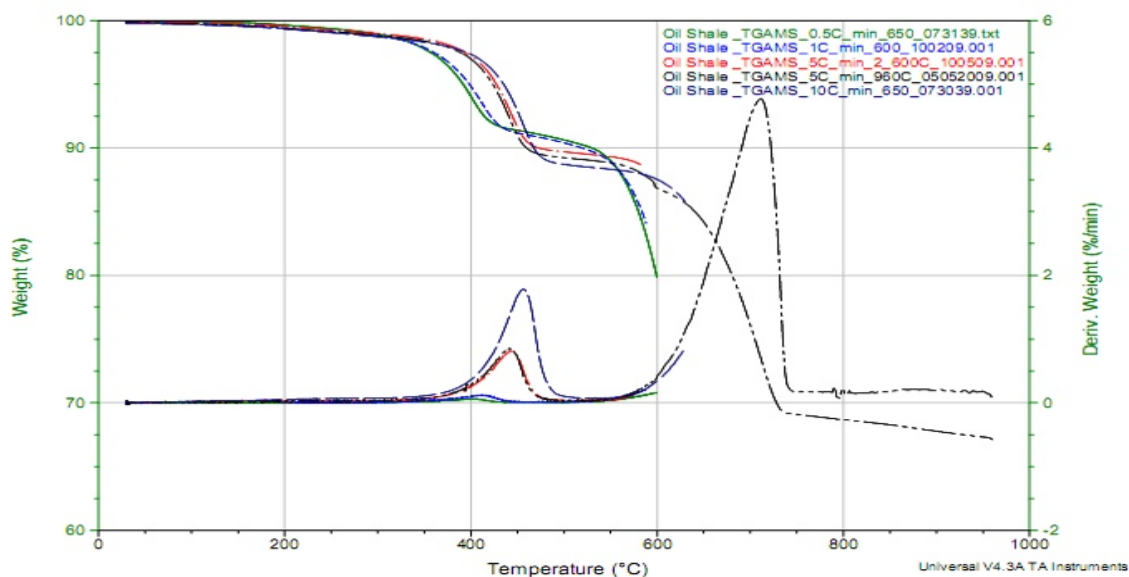


Figure 9: TGA thermograms at different thermal programs.

The advantage of the MS is that it allows for product identification as the process unfolds. As an example, Figure 10 shows the rates of evolution of different products as a function of temperature for a heating rate of 10°C/min. The relative peak intensity is on the y-axis. In each of the compound classes, the lighter components appear ahead of the heavier components, but these differences are minor.

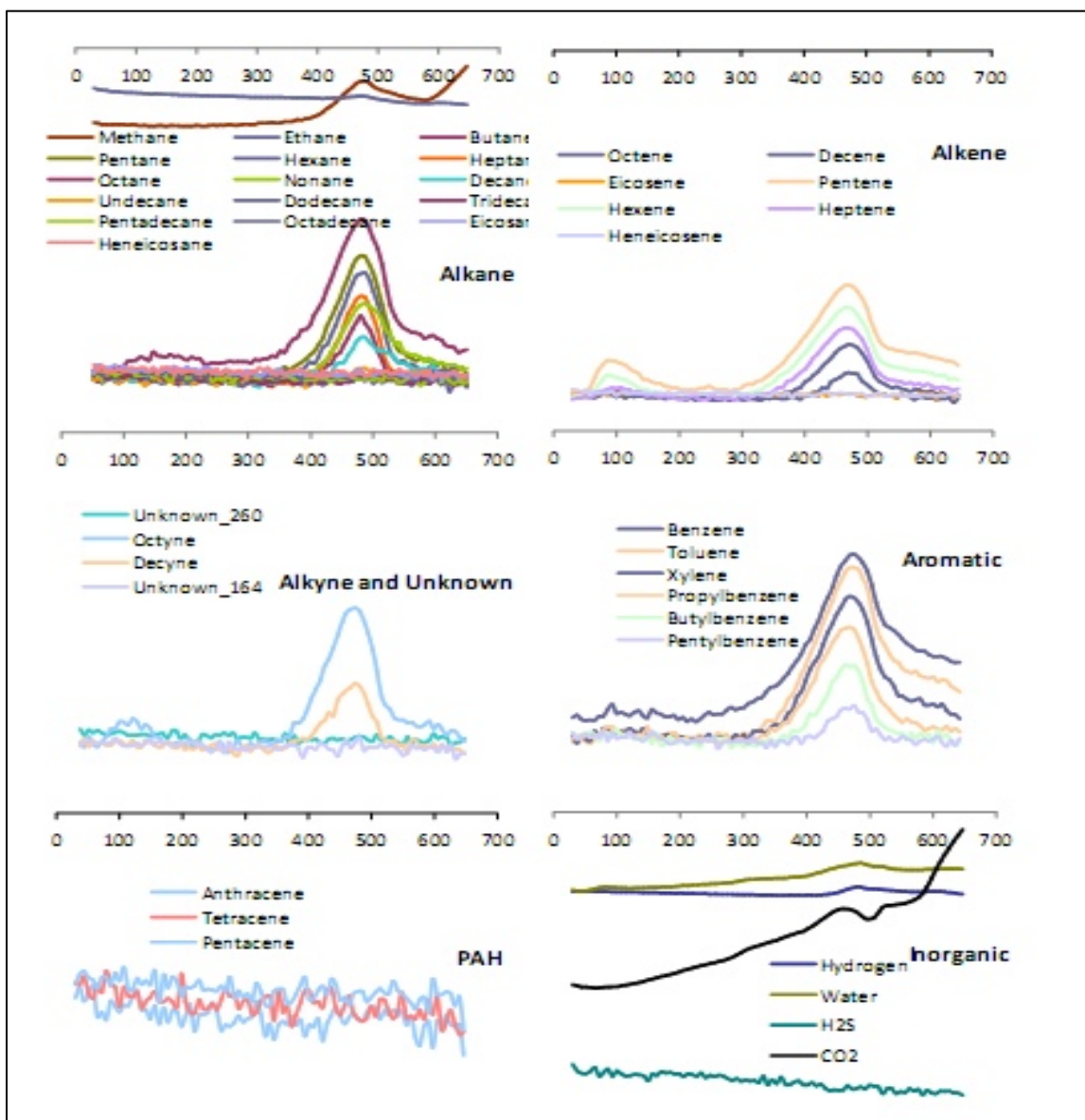


Figure 10: Different classes of compounds identified during pyrolysis of oil shale in a TGA-MS.

The behavior of compounds with the same number of carbons is compared in Figure 11. The peaks for hexane and benzene appear to overlap at two different heating rates. The same observation can be made for saturated, double bonded, and aromatic compounds with 10 carbons.

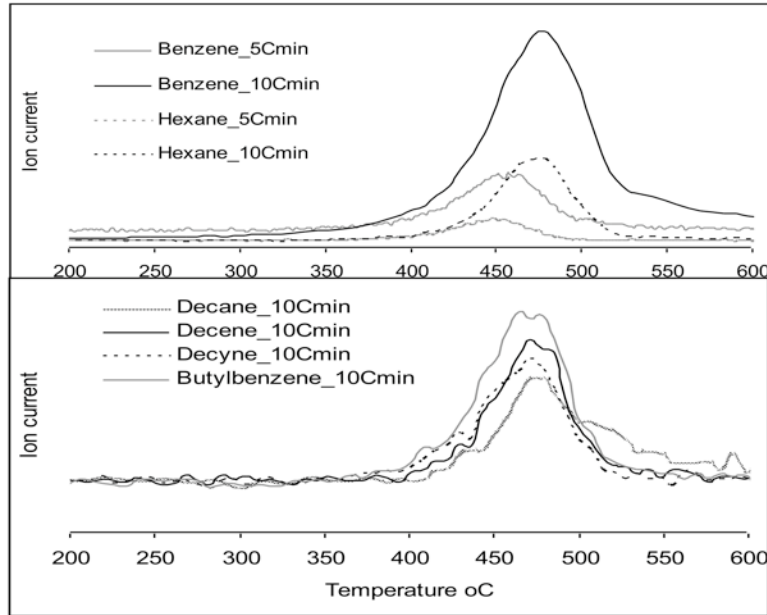


Figure 11: Comparison of the key components on thermal scale at different heating rates.

Subtask 4.4 - Effect of Oil Shale Processing on Water Compositions

The objective of the current work is to analyze the impact of oil shale pyrolysis on water composition for in-situ process development. The project team performed a few water-soak experiments where the oil shale samples were first soaked in water for different durations prior to pyrolysis. Oil samples were collected from the hydrous pyrolysis experiments and compared with the non-hydrous (ordinary) pyrolysis. The gas chromatography (GC) and GC-MS analysis of the water-soaked pyrolysis was reported earlier. There were some changes in the relative compositions of organic species when the two types of experiments were compared; aromatics and alkenes were higher in concentration in hydrous pyrolysis compared to ordinary pyrolysis at the same conditions.

In order to study the changes in water compositions after long-time contact with reacting shale, a high-pressure batch reactor system was constructed as shown in Figure 12. A batch hydrous pyrolysis experiment was performed at 200°C for 24 hrs with 3/4" diameter oil shale core. This particular experiment did not produce any measurable oil. The water in the reactor was collected for further analysis. The sample will be sent to a commercial laboratory to obtain concentrations of dissolved organics. A set of higher temperature reactions at longer durations are under way.

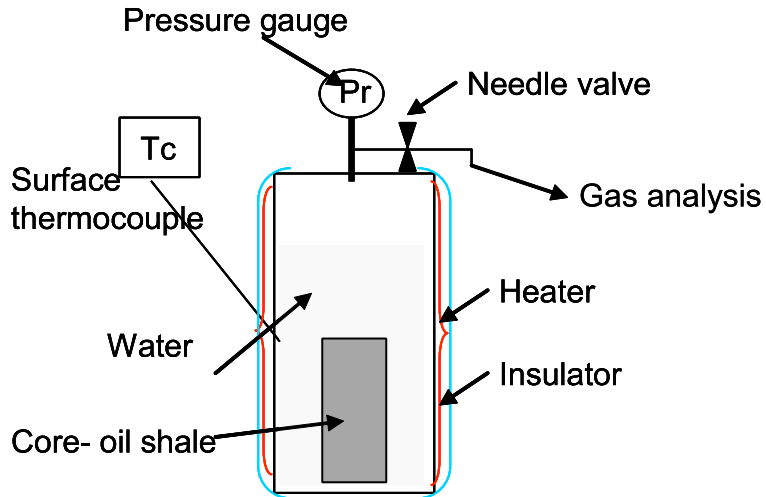


Figure 12: Schematic of the experimental system used for the batch hydrous pyrolysis experiments.

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.

Using a combination of X-ray microtomography (XMT), X-ray nanotomography (XNT), and specialized software, the project team imaged the 3D network of the pores, kerogen/mineral phases, crack network and flow channels of oil shale samples before and after pyrolysis. Figure 13 shows the 3D volume rendered images from the reconstructed multi-scale X-ray CT data for the Mahogany oil shale drill core sample before pyrolysis. The sample was first imaged with traditional XMT at 39 μm voxel resolution, then by high resolution X-ray microtomography (HRXMT) at 1 μm voxel resolution, and finally by XNT at 60 nm voxel resolution. Gray scale levels in Figure 13 indicate variation in the X-ray attenuation coefficients, which depend on the density and atomic number of material within each voxel. Lamellar structures (kerogen-rich layers and silicates-rich layers) are observed. The middle column shows the distribution of the kerogen phase. These results further validate results obtained from optical microscopy. At a voxel resolution of 60 nm (XNT), individual grains can be identified easily. The pore structure of this unreacted material is not clear.

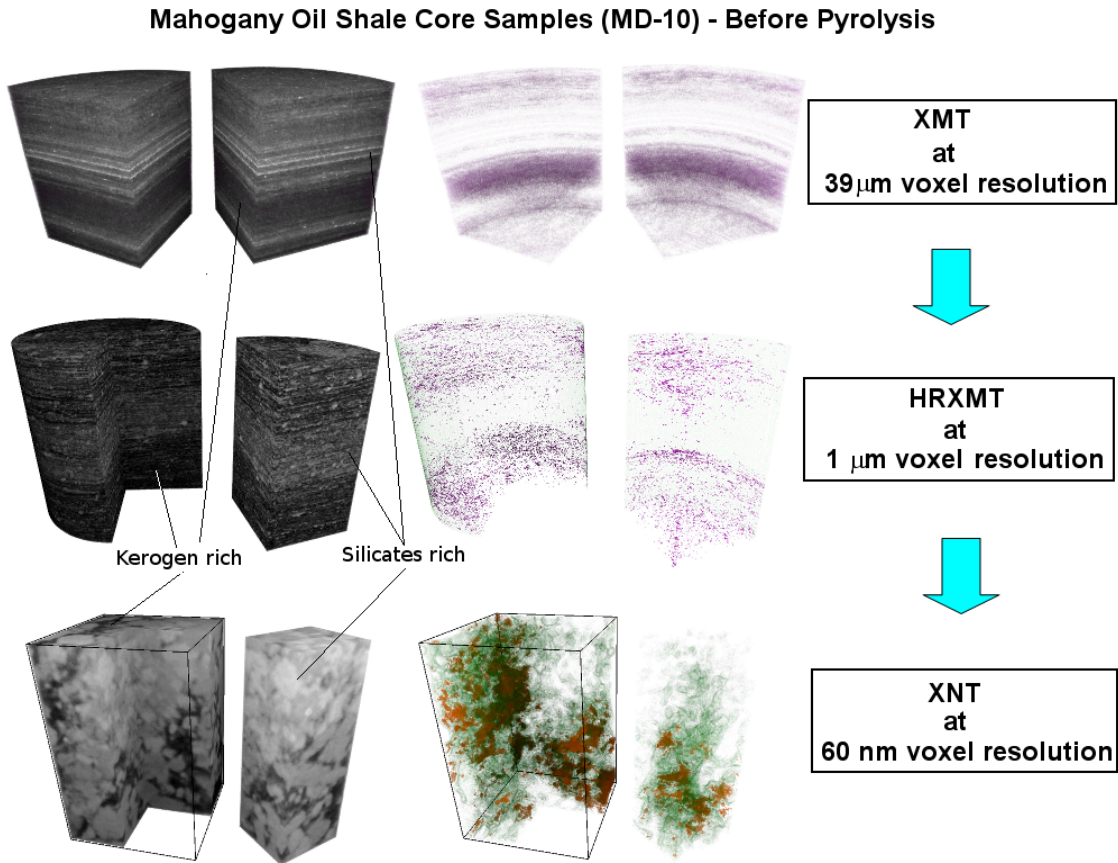


Figure 13: Volume rendered images of Mahogany oil shale drill core sample MD-10 from reconstructions of XMT at 39 μm voxel resolution, HRXMT at 1 μm voxel resolution and XNT at 60 nm voxel resolution. Gray scale level indicates variations in the X-ray attenuation coefficients. Middle column shows distribution of kerogen phase (in purple, purple and brown colors for XMT, HRXMT and XNT, respectively).

The image digitalization of the oil shale sample allowed the project team to obtain the pore network structure that evolved during pyrolysis. Figure 14 shows the 3D volume rendered images from the reconstructed multi-scale X-ray CT data for the Mahogany oil shale drill core sample after pyrolysis (400°C, N₂ flow). 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. Cracks and voids as small as 100 nm (from XNT images) were observed inside region A (silicate-rich lamellar structure). However, larger, anisotropic cracks and voids are developed inside region B (kerogen-rich lamellar structure from HRXMT images) of Figure 14.

Mahogany Oil Shale Core Samples - After Pyrolysis (400 °C)

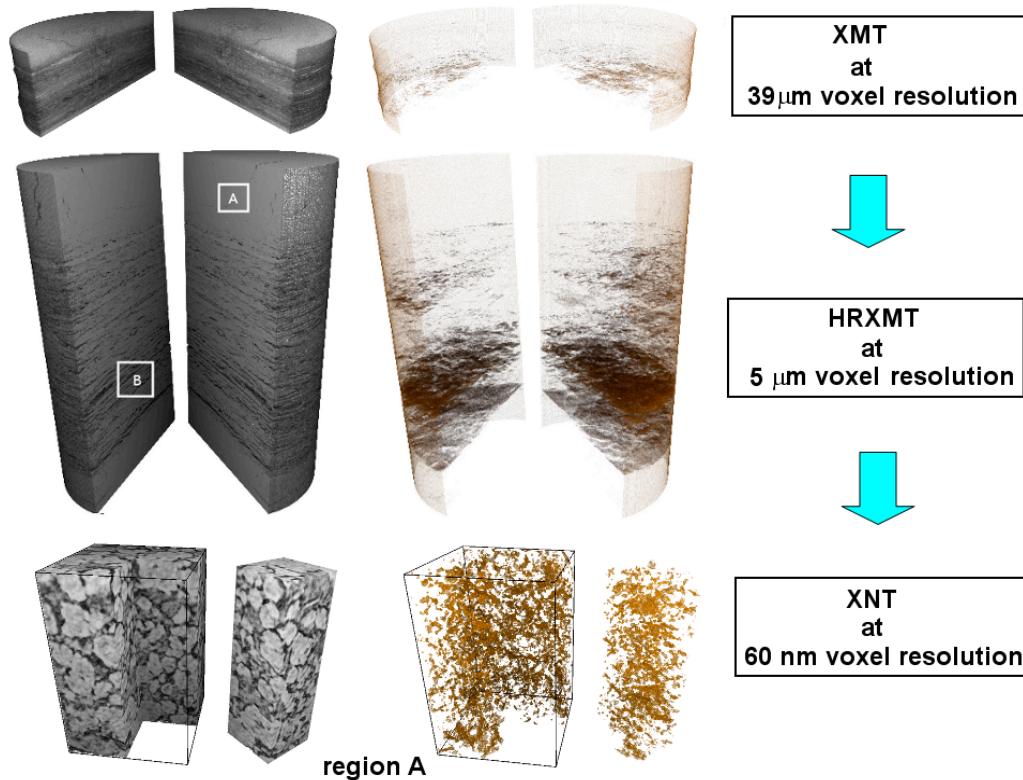


Figure 14: Volume rendered images of Mahogany oil shale drill core sample after pyrolysis (400 °C, N₂ flow) from the reconstructions of XMT at 39 μm voxel resolution, HRXMT at 5 μm voxel resolution and XNT at 60 nm voxel resolution.

As indicated previously, the cracks and voids inside region A (silicate lamellar structure) of the oil shale pyrolysis product are small and are created due to thermal expansion of grain boundaries. Figure 15 illustrates the 3D view of the LB simulation for saturated flow through the pore space of the oil shale after pyrolysis (region A). After removing the solid phases, the right-hand side of Figure 15 shows the nature of the flow channels, e.g. the pore network structure after pyrolysis. The velocity scale is color-coded: solids are white, and solution velocity ranges from black for no flow, through blue, green, yellow and finally red for the highest flow rate. The pore structure deduced from the images was used for LB simulations to calculate the permeability in the pore space of the oil shale after pyrolysis. The estimated permeability from LB simulation of this silicate-rich zone was about 0.00363 μm² or 0.363 mD (millidarcy). However, the absolute permeability is highly anisotropic. Figure 16 shows the 3D views of LB simulated flow along the x-axis through the reconstructed HRXMT image of oil shale pyrolysis product sample (region B). The estimated reacted core permeability in this kerogen-rich zone is 3.87x10⁻⁸ cm² or 3.87 darcy which is four orders of magnitude higher than that in region A.

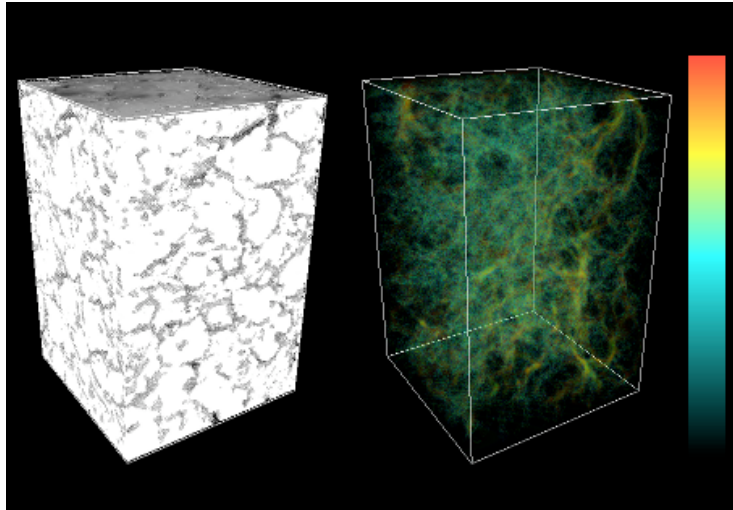


Figure 15: 3D views of LB simulated flow through the reconstructed XNT image of oil shale pyrolysis product prepared at 400°C (region A). Solid phase is white (left). Transparent solid phase (right) reveals flow channels color-coded by velocity. The estimated permeability is $0.000363 \mu\text{m}^2$ or 0.363 mD (millidarcy).

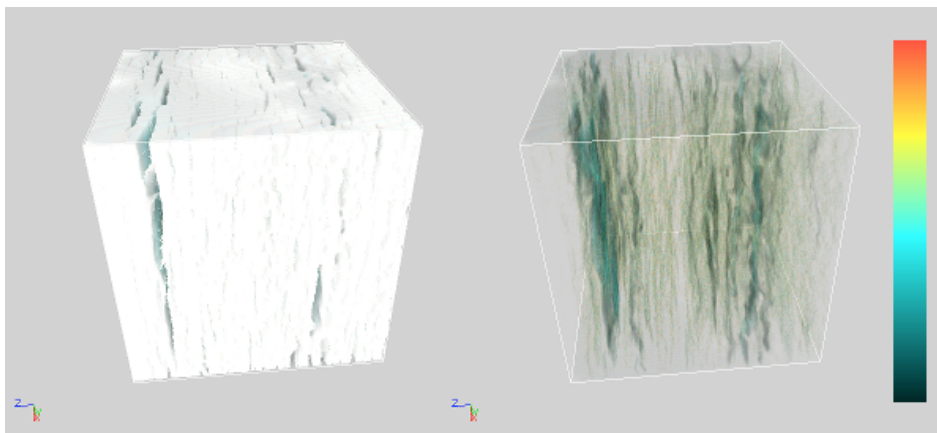


Figure 16: 3D views of LB simulated flow along x-axis through reconstructed HRXMT image of oil shale pyrolysis product (region B) with transparent solid phase to reveal flow channels. The estimated permeability is $3.87 \times 10^{-8} \text{ cm}^2$ or 3.87 darcy.

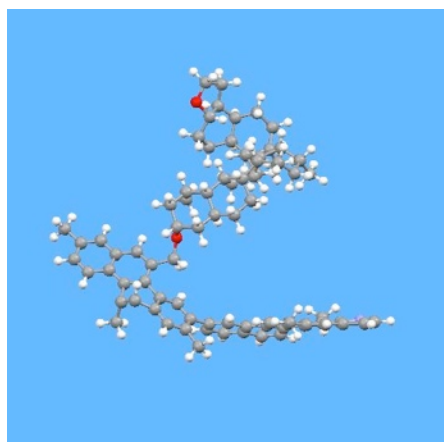
It is evident that XNT imaging will be required to provide satisfactory pore structure information for the silicate-rich zone. Some of the pore space created during pyrolysis is clearly visible at this resolution and it was possible to distinguish between the reaction products and the host shale rock.

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

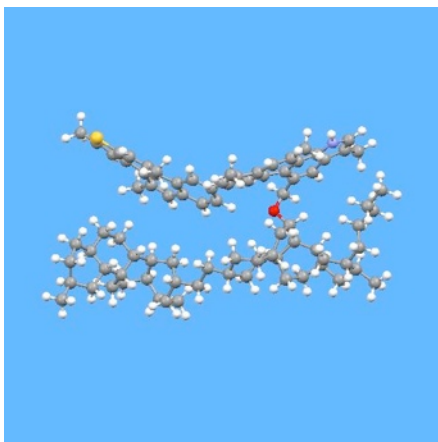
The project team requested permission to use experimentally measured PDFs of an oil shale sample in a paper entitled "Three-Dimensional Structure of the Siskin Green River Oil Shale Kerogen Model: A Computational Study." The private source of the data has denied the permission, so the project team will pursue new measurements of the PDF in a Green River oil shale sample for which there are not IP issues. Work in securing the sample and obtaining the necessary measurements at Argonne National Lab is in progress.

The project team also participated in discussions with the rest of the ICSE in situ thermal processing group to define a series of standard samples, handling protocols and spectroscopic measurements that will be used to guide the modeling work in this subtask. As a consequence of these discussions, the group is working to secure a fresh oil shale core.

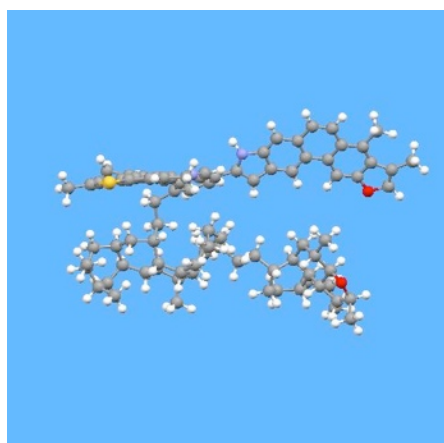
Work has begun on ab initio calculations and molecular dynamics simulation of asphaltenes with the objectives of (1) developing 3D models of asphaltenes based on existing 2D model, (2) studying agglomeration of asphaltenes and (3) studying the interaction between asphaltenes and mineral matter. First, 2D models of several asphaltenes, namely Campana, Mid-Continent U.S., San Joaquin Valley, Loydminster W., Maya, and Heavy Canadian (Siskin et al., 2006) were optimized using GAMESS at the RHF/STO-3G level of theory. In all asphaltene models, the presence of a flexible bridging group connecting the aromatic group with the aliphatic group prompted researchers to re-optimize the 3D structures further to determine the global minima (see Figure 17). For each asphaltene model, the project team found several conformers due to the flexible bridge (either a $-\text{CH}_2\text{O}-$, $-\text{CH}_2\text{CH}_2-$, or $-\text{CH}_2-$ group) between aromatic and aliphatic groups, but only the global minima structures are shown in Figure 17. Undoubtedly, the global minima structures may change in the presence of the mineral matter and/or another asphaltene unit where they are realistically connected. However, for the purpose of studying the agglomeration of asphaltenes where only the bare molecules are involved, minimization of the unattached asphaltene unit is sufficient.



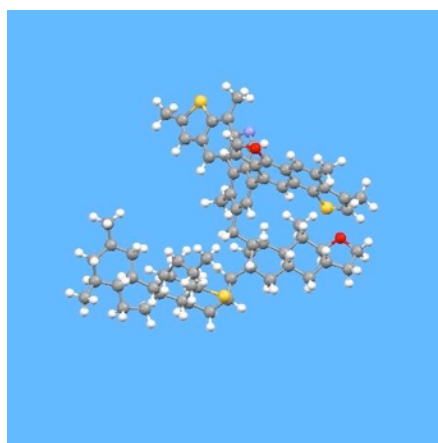
Campana



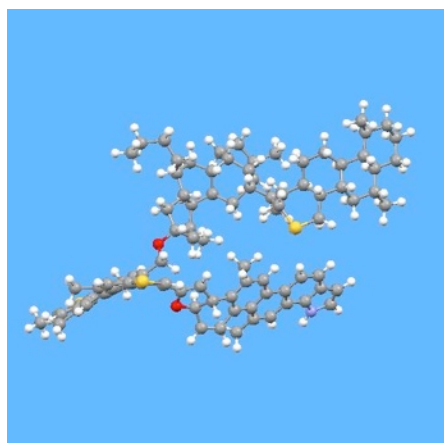
Mid-Continent



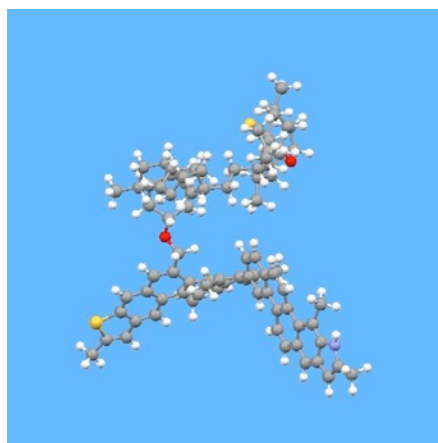
San Joaquin Valley



Loyminster W.



Maya



Heavy Canadian

Figure 17: 3D models of asphaltenes: gray-carbon, red-oxygen, yellow-sulfur, white-hydrogen, blue-nitrogen.

Team members next studied the stacking mechanism of asphaltene agglomeration. First, they performed DFT calculations using the M06-2X functional (Truhlar *et al.*, 2008) on a 3-unit stack of Campana asphaltene to determine the preferred orientation (parallel stack, anti-parallel stack,

or inverted stack). The DFT results suggest that out of the three possible stacking arrangements in the 3-unit models (see Figure 18), the parallel stack is the preferred orientation. This results is due to the stronger π - π interactions where all the aromatic groups are oriented parallel to each other.

Molecular dynamics simulation found in the HyperChem suite of programs are currently underway to determine how the asphaltene molecules stack in bigger models, how many units there are per stack, and how they interact with the mineral matter. Researchers will also study the stacking mechanism of asphaltenes in the presence of solvents (e.g. toluene). Lastly, all the structures will be re-optimized in the presence of the mineral matter.

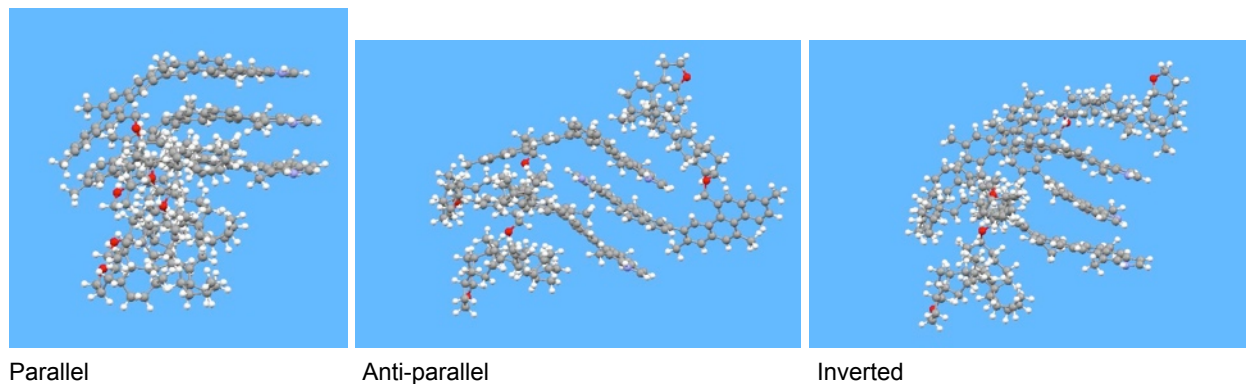


Figure 18: Stacking models in Campana asphaltene: gray-carbon, red-oxygen, white-hydrogen, blue-nitrogen.

Task 5.0 - Environmental, Legal, Economic and Policy Framework

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

The project team continued to monitor and review litigation challenging the federal oil shale leasing rule, the Programmatic 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 team also met with representatives from the U.S. Fish and Wildlife Service and the Utah Division of Wildlife regarding current and foreseeable plant and wildlife issues that could complicate energy development. Team members reviewed documents regarding the U.S. Fish and Wildlife Service's decision to protect sage grouse under the Endangered Species Act listing and researched the decision's implications. The team monitored the 2010 Utah legislative session, including reviewing pending bills, attending committee meetings, reviewing committee testimony, and conducting related legal research. Work also began on an outline of the Topical Report on land and resource management issues relevant to in-situ thermal process deployment during this quarter.

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

The project team completed and submitted a Topical Report entitled "Policy Analysis of Water Availability and Use Issues For Domestic Oil Shale and Oil Sands Development." As part of finalizing that report, team members updated research on water consumption for oil shale and oil sands development, water rights previously issued for oil shale and oil sands development,

water resources potentially available to support oil shale and oil sands development, existing water quality concerns affecting oil shale or oil sands development within Utah, water quality regulations and standards, discharge permitting, and regulatory developments regarding hydraulic fracturing. Team members also met with representatives from the Government Accountability Office regarding water for oil shale development. Work also began on an outline of the Topical Report on produced water management.

6.0 – Economic and Policy Assessment of Domestic Unconventional Fuels Industry

Subtask 6.1 Engineering Process Models for Economic Impact Analysis

The project team had a milestone scheduled for completion in this quarter of identifying and describing selected scenarios and the methodology applied to obtain associated upstream supply costs. A description of the scenarios and of the methodology used for the economic analysis of various heavy oil production methods and subsequent upgrading methods are explained in this report.

Develop Scenarios for Economic Evaluation

The scenarios include:

- Piceance Basin Oil Shale Extraction
 - Surface mining
 - In situ extraction
- Unita Basin Tar Sands Extraction
 - Surface mining
 - In situ extraction
- North Slope Heavy Oil Extraction
 - Steam Injection and oil well extraction

Each scenario will be developed at a production capacity of 50,000 bbl/d and will include one or more types of extraction with the subsequent upgrading of the crude oil using primary upgrading followed by secondary upgrading to make oil of a quality that can be pipelined from the point of upgrading to a refinery capable of refining it. Not all refineries are capable of processing heavy oils with their inherently high concentrations of nitrogen, sulfur and heavy metals. Fortunately for the Piceance and Uinta Basin resources, the refineries in Salt Lake City and Denver have the capability of processing heavy oils as they are presently operating on Athabaskan crude oil derived from heavy tar sands.

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. Primary upgrading of surface mined oil shale is via a retort followed by washing with hot water to remove water soluble salts. Primary upgrading of surface mined tar sands consists of the separation of the sand from the oil followed by washing with hot water to remove the water soluble salts. With the other extraction methods, simply washing with hot water to remove water soluble salts is all that is needed. A coker is used for primary upgrading for very heavy oils. 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 NH₃, and heavy metals. The hydrogen needed for hydrotreating is considerable, e.g. 350 m³ H₂ per m³ shale oil (S.G. 0.911). This 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. All scenarios include transport of the crude oil to a refinery for further processing.

Develop Supply Costs for Scenarios

Supply costs are being developed for the various scenarios using industrial standard methods for the estimation of capital and operating costs for each year over the life of the project. Standard accounting methods are used to establish discounted cash flow predictions for the project allowing various measures of profitability to be established. Operating costs are determined by accounting for 1) the direct manufacturing costs including feed stocks, utilities (electricity and water for steam, cooling and process), refrigeration, fuels, solid waste treatment, waste water treatment and air-pollution abatement as well as labor and maintenance, 2) operating overhead, and 3) fixed costs including property taxes/insurance and depreciation as well as general expenses including selling (or transfer) expenses, research (direct or allocated) expenses, administrative expenses and management incentives. Well drilling cost are estimated from recent industrial data available from collaboration with industry. The project team will use a mixture of capital costing methods for this project including:

1.) Method of Hill (1956)

To produce an estimate, only two things are needed: a production rate and a flow sheet. The flow sheet must show the major pieces of equipment including gas compressors, reactors and separation equipment. Heat exchangers and pumps are not considered in making the estimate. The estimate uses the Marshall Stevens Process Industry Average Cost Index to account for inflation in this industry. Different types of processes, e.g. fluid vs. solids handling, have different cost estimating factors. Additional factors to account for site preparation, services facilities, utility plants and related facilities can be added. The estimate is accurate to approximately $\pm 50\%$ and is particularly useful for low-pressure petrochemical plants.

2.) Method of Lang (1947a,b and 1948 with improvements by Peters and Timmerhaus, 1968)

This method requires a process design, complete with a mass and energy balance and equipment sizing. The estimate uses overall factors that multiply estimates of the delivered cost of all the process equipment including heat exchangers, pumps, gas compressors, reactors and separation equipment. Important factors account for the effects on unit cost of materials of construction, operating pressure and delivery costs of the equipment. The estimate uses the Marshall Stevens Process Industry Average Cost Index to account for inflation in this industry. Different types of processes, e.g. fluid vs solids handling, have different cost estimating factors. Using various Lang factors, either the total permanent investment (fixed capital investment) or the total capital investment (including working capital at 17.6% of total permanent investment) can be determined. The estimate is accurate to approximately $\pm 35\%$.

3.) Method of Guthrie (1969 and 1974)

The method requires an optimal process design with mass and energy balances, equipment sizing, selection of materials of construction and a process control configuration. As with the Lang method, the Guthrie method is applied by estimating the f.o.b purchase cost of each piece of equipment. Instead of using an overall factor to account for installation of the equipment and other capital costs, individual factors for each type of equipment are used. For example, the materials of construction can be different for a reactor or separation unit. The components of total permanent investment including contingency and contractor fees, site development costs, building costs, and offsite facility costs are added to the

summation of installed equipment costs. The total permanent investment is added to the working capital to determine the total capital investment. The estimate uses the Chemical Engineering Cost Index to account for inflation by equipment type in this industry. The estimate is accurate to approximately $\pm 20\%$.

A scenario similar to one of those under investigation in this work was done in the 1980's, and there is not enough additional information to improve upon the processing route. In this case, the capital costs have been updated for a new production rate and a 2010 purchase date using the method of Hill, and the operating costs have been updated to modern unit operation costs. In all other cases, the capital costs have been estimated by the Guthrie method where possible or the Lang method where not. The annualized cost of the capital investment is determined over the life of the plant giving an annualized capital expense. This expense is added to the annual operating costs for the plant to determine the annual cost for producing the annual production of the plant. The annual cost divided by the annual production rate of the plant gives the supply cost for that year. Making assumptions about the sales price for the crude oil to the refinery and its price sensitivity, the pre-tax profit from the production and upgrading operations developed for these scenarios will be determined as well as the depreciation, depletion and income taxes for these operations. Finally, various rigorous profitability measures like annual cash flow, annual net present value and investor's rate of return will be determined for each scenario.

Subtask 6.2 - Policy analysis of the Canadian oil sands experience

The project team continued research and analysis of the relevance of policy and public perception to the development of a domestic oil sands industry. The team also reviewed and began drafting analysis of research related to the realities and perceptions of the carbon footprint of oil sands development in Canada. Team members attended a presentation on the environmental and economic aspects of the Canadian oil sands given by the Canadian Consul General. The team also began researching royalty and investment issues relevant to development of the Canadian oil sands and the federal and state counterparts in the United States in support of deliverables for next quarter.

Subtask 6.3 – Market Assessment Report

The project team had a milestone this past quarter to identify and describe the methodology applied to assess impact of downstream market conditions on potential revenue from upstream scenarios. For the hypothetical, non-integrated oil producers considered in this Assessment, the downstream risk to revenue is related to the uncertainty concerning the future path of the price they receive from refiners. Team members are accounting for such oil price risk using a model of the price of the West Texas Intermediate (WTI) marker crude. The parameters of this model are established from oil price data but may also be tuned to reflect "what if" scenarios for the level and volatility of the future prices of oil.

An option available to unconventional oil producers is to invest in the facilities necessary to upgrade the crude to near the quality of the marker. In this case, the oil price risk to the producer is accurately measured using the marker price. To the extent the crude is produced to a different quality, the producer is also subject to a "price differential" risk, arising out of discounts and premia of the produced grade of crude to that of the marker crude. How the risk of the discounted/premium price compares to the risk of the marker price depends on the particular grade of produced crude and on the correlation between the marker price and the discounted/premium price. Team members are using a time-series analysis of various crude streams (differentiated by location of origin and physical properties) which measures price correlation and disaggregates the price differentials into components based on physical properties of the crude such as API, sulfur, and nitrogen.

Ultimately, this part of the Assessment provides a measure of the oil price risks attending different resources and different technologies employed to produce from the resources.

The project team has also been evaluating issues related to the microeconomic (supply cost) and macroeconomic (economic impact) analyses of these scenarios. On the supply cost side, unconventionally produced crude suffers from economic, legal, and political uncertainties, which tend to inhibit private investment. Economic uncertainties can be divided into those that affect the costs and those that affect the benefits of unconventional crude production. Some inputs, at their expected cost, are more important determinants than others of the supply cost of crude. Independently, some costs (e.g. natural gas) are more volatile than others. The team's analysis accounts for the uncertain future price of natural gas using a family of probability models, similar to what is being done with the oil price risk on the revenue side as described above.

The Assessment does not make an account for the cost associated with negative externalities ("public costs") stemming from, for example, air quality or greenhouse gas emissions. Neither does the Assessment make an account for the positive externalities ("public benefits") associated with, for example, lower costs to future producers from the learning experience of pioneer producers or any reduction in vulnerability to crude oil macroeconomic shocks from a lower share of imported crude attending a more rapid increase in domestic production than increase in domestic consumption.

On the economic impact side, development of unconventional fuels could create new jobs, income, and revenue to both the host states and the nation. The Assessment estimates the magnitude of such economic benefits for Utah. The team's approach to estimating economic impacts is input-output analysis, in which both jobs and income directly due to production and jobs and income indirectly due to development by the overall increase in economic activity spurred on by development are counted.

An important uncertainty in the magnitude of such economic benefits is related to the timing of development. If development occurs during a time in which significant labor and capital resources are unemployed, then generally a higher fraction of the jobs and income associated with production is "new" income, rather than jobs and income that come from elsewhere in the macroeconomy.

CONCLUSIONS

The Clean and Secure Energy from Domestic Oil Shale and Oil Sands Resources program hosted a public forum on energy and visits from industry and national laboratories. Research work was focused on four main areas. In the area of oil shale and sands utilization with CO₂ management, CO₂ emissions reductions achievable by converting to oxy-firing in a refinery were estimated and preliminary simulations for a laboratory-scale process heater firing oxy-gas were conducted. 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 fresh oil shale core obtained from Utah's Uinta Basin and developing geologic, kinetic, porosity, and atomistic models that can be applied to a reservoir-scale process. In the area of environment and policy, a topical report entitled "Policy Analysis of Water Availability and Use Issues For Domestic Oil Shale and Oil Sands Development" was released. In the market assessment area, the methodologies used for the economic analysis of various heavy oil production and upgrading methods and for the assessment of the impact of downstream market conditions on potential revenue from upstream scenarios were explained.

COST STATUS

Baseline Reporting Quarter	Yr. 1							
	Q1		Q2		Q3		Q4	
	7/1/09 - 12/31/09		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	331,481	751,634		751,634		751,634
Non-Federal Share	29,456	29,456	131,875	161,332		161,332		161,332
Total Incurred Costs	449,609	449,609	463,356	912,966	0	912,966	0	912,966
Variance								
Federal Share	64,575	64,575	153,247	217,822	0	702,550	0	1,187,276
Non-Federal Share	91,796	91,796	-10,623	81,172	0	202,424	0	323,678
Total Variance	156,371	156,371	142,624	298,994	0	904,974	0	1,510,954

Baseline Reporting Quarter	Yr. 2			
	Q5		Q6	
	10/1/10 - 12/31/10		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		751,634		751,634
Non-Federal Share		161,332		161,332
Total Incurred Costs	0	912,966	0	912,966
Variance				
Federal Share	0	1,510,679	0	1,834,081
Non-Federal Share	0	404,513	0	485,347
Total Variance	0	1,915,192	0	2,319,428

MILESTONE STATUS

There were 10 milestones/deliverables scheduled for completion in this quarter. The milestone in Task 2.0, Technology Transfer and Outreach, was to upload the geodatabase of water information to the interactive map. This milestone was completed and reported in the Task 2.0 summary above.

Subtask 3.1, the macroscale CO₂ analysis, had a milestone of identifying and collecting experimental, literature, & simulation data on GHG emissions from process heaters. The project team has completed this milestone and integrated some of this baseline data into Figure 1 of this report.

Subtask 4.1, which focuses on the development of CFD-based simulations tool for in situ thermal processing of oil shale/sands, had two milestones. The first was to implement porosity and DQMOM for porous fixed bed into the ARCHES simulation tool. The second was to implement submodels for kinetics of oil shale pyrolysis, porosity development, etc. that are consistent with available experimental data. However, as described in the Subtask 4.1 summary above, there has been a change of direction in this subtask due to the determination by project researchers that the simulations tools employed needed to account for the actual geometry of the pieces of shale in the bed. A suite of commercial software tools has been identified and employed in accomplishing this task including EDEM, GAMBIT, Matlab, and Star-CCM+. Due to the change in direction, a new set of milestones is suggested that will better indicate the progress of the development of the CFD-based simulation tool:

1. Implementation of correct geometry representation in Star-CCM+ (June 2010)
2. Implement submodels for s pyrolysis, porosity development, etc. that provide a stable solution (September 2010)
3. Topical report describing completed validation/uncertainty quantification analysis of Ecoshale capsule that does not violate contract with Red Leaf for data sharing (December 2010)

The subtask 4.2 milestone was to select a dataset for use in validation/uncertainty quantification of in-situ production models. This dataset has not yet been identified, but team members are hopeful that a relevant dataset from either an oil sands or oil shale company will be identified in the near future. In the meantime, the cross section data that is being built by UGS as part of the subtask is an essential piece that goes into the reservoir models. In subtask 4.3, the multiscale pyrolysis project, the milestone was to complete pyrolysis experiments at two different scales. The project team has completed numerous experiments with crushed samples (grain scale) and 3/4- and 1-inch cores; some grain scale experiments are reported in the subtask 4.3 summary above. This two-scale system has not yet been thoroughly analyzed, but the team does now have the data. Subtask 4.6, the kerogen/asphaltene/mineral matrix project, has a milestone to develop 3D models of kerogen and asphaltenes based on existing 2D models. The literature review of existing 2D models for both kerogen and asphaltenes has been completed. The 3D models for kerogen have been finalized and were reported in the quarterly report from the fourth quarter of 2009. The 3D models for asphaltenes are currently being finalized as reported in the subtask 4.6 summary above.

The milestone for subtask 5.2, a topical report submitted to DOE/NETL addressing issues and analysis of water availability for oil shale/sands development, was completed with the submission of the report entitled "Policy Analysis of Water Availability and Use Issues For Domestic Oil Shale and Oil Sands Development" by John Ruple and Robert Keiter. This topical report was submitted to NETL on March 31, 2010.

For subtask 6.1, engineering process models for economic impact analysis, the milestone was to identify and describe selected scenarios and the methodologies applied to obtain associated upstream supply costs. This milestone has been completed with the summary provided above for subtask 6.1. The subtask 6.3 milestone, to identify and describe the methodologies applied to assess the impact of downstream market conditions on potential revenue of upstream scenarios was provided in this report.

NOTEWORTHY ACCOMPLISHMENTS

For the basin-wide characterization part of subtask 4.2, a preliminary synthesis and sequence stratigraphic model has been constructed across the Uinta Basin. This model will be further tested, revised, and refined with analysis of additional core. In subtask 4.5, the anisotropic features of oil shale permeability have been quantified and may be the first reported 3D imaging of pyrolyzed oil shale by HRXMT and XNT.

PROBLEMS OR DELAYS

The necessity and utility of XNT for imaging oil shale has been demonstrated in subtask 4.5. It is clear that access to a Nano CT facility is necessary. Funds should be sought for purchasing and installation at the University of Utah. As noted in the summary for subtask 4.6 above, the publication of the manuscript “Three-Dimensional Structure of the Siskin Green River Oil Shale Kerogen Model: A Computational Study” has been delayed due to the complications in obtaining experimental data.

RECENT AND UPCOMING PRESENTATIONS/PUBLICATIONS

C. H. Hsieh, C. L. Lin and J. D. Miller, “Pore scale analysis of oil sand/oil shale pyrolysis by X-ray Micro CT and LB simulation.” Poster presented at SME Annual Meeting, Phoenix, AZ, February 28 – March 3, 2010.

Ruple, John C.; Keiter, Robert B. Water for commercial oil shale development in Utah: Allocating scarce resources and the search for new sources of supply, *Journal of Land, Resources & Environmental Law* **30(1)** (2010), pp. 95-143.

Ruple, John C.; Keiter, Robert B. Water for commercial oil shale development in Utah: Clarifying how much water is needed and available, *Journal of Energy & Natural Resources Law* **28(1)** (2010), pp. 49-86.

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 presented at 2010 AAPG Annual Meeting, New Orleans, LA, April 12, 2010.

K. E. Kelly, J. Dumas, A. F. Sarofim, and D. W. Pershing, “Evaluating opportunities for reducing life-cycle, well-to pump GHG emissions from conventional and unconventional fuels.” Poster presented at University of Utah Unconventional Fuels Conference, Salt Lake City, UT, April 28, 2010.

Jennifer Spinti, Philip J. Smith, and Brandon Hochstrasser, “Oxy-gas process heaters for efficient CO₂ capture.” Poster presented at University of Utah Unconventional Fuels Conference, Salt Lake City, UT, April 28, 2010.

Benjamin Isaac and Philip J. Smith, "Development of CFD-based simulations tool for in situ thermal processing of oil shale/sands." Poster presented at University of Utah Unconventional Fuels Conference, Salt Lake City, UT, April 28, 2010.

C. H. Hsieh, C. L. Lin and J. D. Miller, "Pore scale analysis of oil sand/oil shale pyrolysis by X-ray Micro CT and LB simulation." Poster presented at University of Utah Unconventional Fuels Conference, Salt Lake City, UT, April 28, 2010.

Lauren P. Birgenheier, "Geologic characterization of Utah oil shale deposits," University of Utah Unconventional Fuels Conference, Salt Lake City, UT, April 28, 2010.

Jacob Bauman and Milind Deo, "Modeling in-situ production of shale oil from the Green River oil shale in the Uinta Basin." Poster presented at University of Utah Unconventional Fuels Conference, Salt Lake City, UT, April 28, 2010.

Pankaj Tiwari and Milind Deo, "Multiscale thermal processing (pyrolysis) of oil shale." Poster presented at University of Utah Unconventional Fuels Conference, Salt Lake City, UT, April 28, 2010.

Robert Lee Krumm, Pankaj Tiwari and Milind Deo, "Effect of oil shale processing on water compositions." Poster presented at University of Utah Unconventional Fuels Conference, Salt Lake City, UT, April 28, 2010.

I.S.O. Pimienta, A.M. Orendt, R.J. Pugmire, and J.C. Facelli, "Atomistic modeling of oil shale kerogen and asphaltenes." Poster presented at University of Utah Unconventional Fuels Conference, Salt Lake City, UT, April 28, 2010.

John Ruple and Robert Keiter, "Clean and secure energy from Utah's oil shale and oil sands resources: Environmental, legal and policy framework." Poster presented at University of Utah Unconventional Fuels Conference, Salt Lake City, UT, April 28, 2010.

Benardo Castro, Milind Deo, Michael Hogue, Kerry Kelly, Terry Ring, Jennifer Spinti, Kirsten Uchitel, Jon Wilkey, "Unconventional fuels market assessment." Poster presented at University of Utah Unconventional Fuels Conference, Salt Lake City, UT, April 28, 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," *Flow Measurement and Instrumentation*, accepted for publication.

Jennifer P. Spinti, Jeremy N. Thornock, and Philip J. Smith, "Oxy-gas combustion for efficient CO₂ capture: Effect of near burner mixing on velocity and composition fields," Mixing XXII, Victoria, BC, Canada, June 20-25, 2010.

K. E. Kelly, A. F. Sarofim, and D. W. Pershing, "Opportunities for reducing CO₂ emissions from conventional and unconventional fuels using oxyfiring: A life-cycle perspective," AFRC International Pacific Rim Combustion Symposium, Maui, HI, September 26-29, 2010.

C. L. Lin, J. D. Miller, C. H. Hsieh, P. Tiwari and M. D. Deo, "Pore scale analysis of oil shale pyrolysis by X-ray CT and LB simulation," 6th World Congress on Industrial Process Tomography, Beijing, China, September 2010.

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

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