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 2011)

Submitted by:
Institute for Clean and Secure Energy
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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

Prepared for:
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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 held a Project Review meeting on the University of Utah campus and began planning the 2011 Unconventional Fuels Conference and field trip. In addition, researchers in the various subtasks submitted topical reports and papers to complete required deliverables.

Subtask 3.1 researchers refined and updated their evaluation of the life-cycle greenhouse gas (GHG) emissions for the air-fired and oxy-fired scenarios developed under Subtask 6.1. From a GHG standpoint, the most attractive scenario appears to be Utah ex situ oil sands production using oxy-firing. Subtask 3.2 researchers performed simulations of both air-gas and oxy-gas burners using the same computational domain and burner geometry. The results show the large temperature and radiative heat transfer increases that are seen in moving from air-firing to oxy-firing, even when flue gas recycle is employed to moderate temperatures in the oxy-fired system.

The Subtask 4.1 team successfully created and performed simulations on an extended geometry domain that more closely resembles the experimental geometry used by Red Leaf Resources. They show a strong influence of boundary conditions on the thermal distribution inside the rubblized shale capsule, the importance of well-insulated boundaries to maximize the heat transfer to shale, and the improvement to heat transfer that occurs when the heating element is placed as low in the capsule as possible. The Subtask 4.2 team completed a Topical Report (submitted to OSTI) that summarized their regional four-core oil shale cross section work. Subtask 4.3 researchers evaluated the effect of particle size and gas flow rate on thermogravimetric analyzer (TGA) thermograms. Mass transfer effects are eliminated with small particle sizes (<70 mesh) and high gas flow rates (100 ml/min). Work by the Subtask 4.4 team showed that for both hydrous and non-hydrous pyrolysis, most of the targeted organic compounds, including the potential aromatics, were below the detection limit of the instrument in all water samples tested. The Subtask 4.5 team completed a Topical Report (submitted to OSTI) summarizing results from micro computed tomography and Lattice Boltzmann simulation analysis of the pore network structure in pyrolyzed oil shale samples. Subtask 4.6 researchers calculated the NMR data for previously modeled kerogen, simulated the pyrolysis of the previously modeled Campana asphaltenes, and began data collection from the Advanced Photon Source at Argonne National Lab. Work began on Subtask 4.7 with the creation of fabrication drawings for a triaxial pressure vessel to be used in studies of the geomechanical reservoir state of oil shale resources.

Subtask 5.1 researchers, working with the University of Utah's Digitally Integrated Geographic Information Technologies Lab, obtained public land inventory and management data from the BLM and categorized land management requirements. In addition, they reviewed publications regarding the prerequisites for effective resource management collaboration. For Subtask 5.2, team members researched the historic development of and recent updates to legal requirements applicable to surface water management, groundwater management, and conjunctive water management.

In Task 6.0, ICSE researchers focused on the completing the seven sections of the draft Market Assessment report, sending these sections out to reviewers, and continuing to revise the engineering and economic analyses for the three in situ development scenarios. In addition, researchers completed research and analysis related to taxes and royalties levied on oil sands production, as well as downstream and marketing challenges facing oil sands development.

PROGRESS, RESULTS, AND DISCUSSION

Task 1.0 - Project Management and Planning

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

Task 2.0 -Technology Transfer and Outreach

This task focuses on industry, academic and public outreach and education efforts, as well as implementing the External Advisory Board (EAB) recommendations. Planning began in earnest this quarter for the 2011 University of Utah Unconventional Fuels Conference, which will be help on Tuesday, May 17, on the campus of the University of Utah. This year, a Uinta Basin field trip component was added to the conference. The field trip will run from May 18-19 with an overnight stay in Vernal, UT. A conference agenda and field trip itinerary are included in Appendix A of this report.

A DOE Project Review Meeting was held on March 10-11 on the University of Utah campus. Olayinka Ogunsola from DOE and Robert Vagnetti from DOE/NETL joined ICSE researchers for a day and a half of presentations and questions. A total of 14 presentations were given. A copy of the meeting agenda is included in Appendix B of this report.

Preparations continued this quarter for the 2011 EAB meeting, which has been delayed from May 2011 to later in the year, and for the 2011 Energy Forum, which has been set for September 14, 2011.

Task 2.0 work this past quarter has also focused on completing the transitioning of the Digital Repository. The Marriott Library at the University of Utah has agreed to permanently house what are now the contents of the ICSE Digital Repository. Additional work was required on the computer program developed to convert the export format of DSpace to a suitable input format for the Marriott Library's ContentDM. The Institute has completed delivery of the Digital Repository contents to the Marriott Library; however, library staff has not yet completed its review of the migration.

Task 3.0 - Clean Oil Shale and Oil Sands Utilization with CO_2 Management

Subtask 3.1 – Macroscale CO_2 Analysis (PI: Kerry Kelly, David Pershing)

During this quarter, the Project Team refined and updated their evaluation of the life-cycle greenhouse gas (GHG) emissions for the air-fired and oxy-fired scenarios developed under Subtask 6.1. They added GHG emissions associated with the diesel vehicles that are used to extract oil sands and oil shale in the ex situ scenarios. In addition, as the Subtask 6.1 scenario results continue to be refined, the investigators continue to update their emission estimates.

Figure 1 shows the most recent GHG emission profiles for the oxy- and air-fired oil sands and shale scenarios developed under Subtask 6.1. The most attractive scenario from a GHG standpoint appears to be the Utah ex situ oil sands production using oxyfiring. The GHG emissions from ex situ oil shale production appear to be low compared to literature data while those for in situ oil shale production appear to be greater. The Project Team is working with Subtask 6.2 investigators to identify possible causes for these differences, keeping in mind that because oil shale is not produced commercially, high levels of uncertainty exist in the literature data. Both the in situ and ex situ oil sands emissions appear to be in the range of literature values.

Subtask 3.1 investigators have begun organizing their results for a topical report or publication but are waiting for final results from Subtask 6.1 before moving forward.

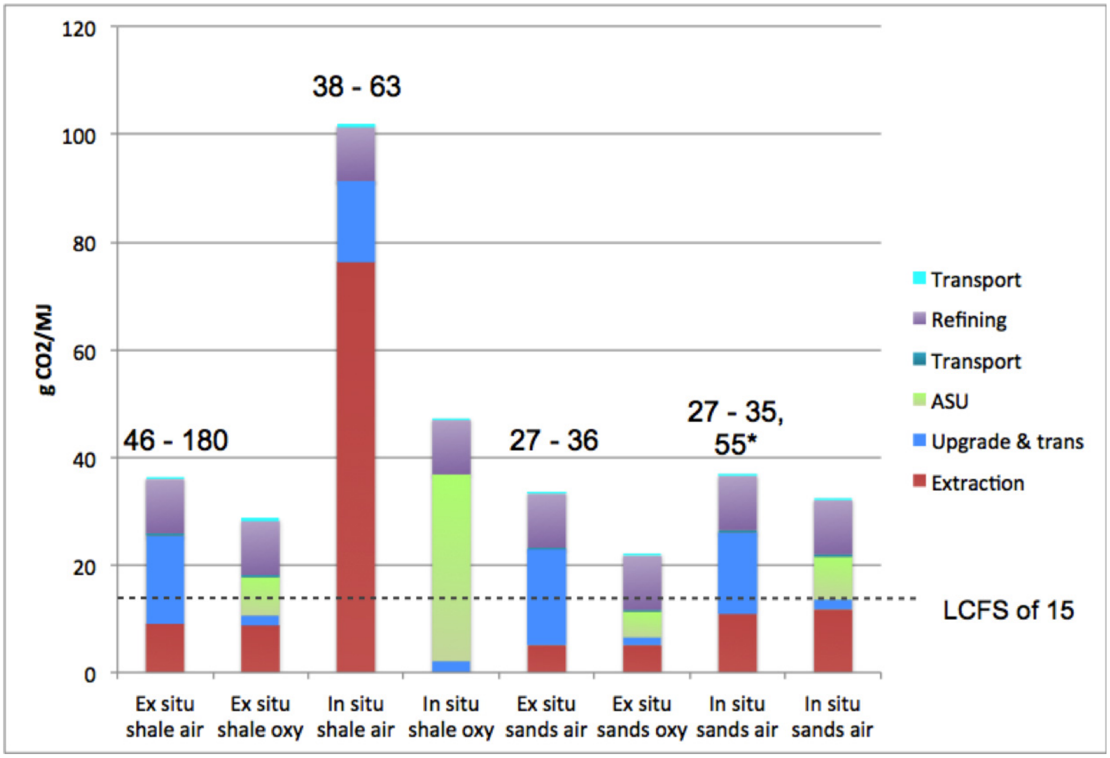


Figure 1: Well-to-pump GHG emissions (extraction, upgrading, transportation, air separation, and refining) for Subtask 6.1 scenarios. The numbers above the bars indicate ranges of GHG emissions for similar processes reported in the literature. The dotted line shows California's low-carbon fuel standard.

Subtask 3.2 - Flameless Oxy-gas Process Heaters for Efficient CO_2 Capture (PI: Jennifer Spinti)

In this quarter, Subtask 3.2 researchers completed simulations of both oxy-gas and air-gas experiments conducted by the International Flame Research Foundation (Coraggio and Laiola, 2009). For both the oxy-gas and air-gas simulations, the same computational domain (2m x 2m x 2m), mesh resolution (225 x 225 x 225), and burner geometry (three concentric injection ports) were used. All transport equations were solved with second order numerical schemes.

Figures 2 and 3 show volume-rendered images of the temperature field for the air-gas and oxy-gas flames respectively. Also shown in the two figures is the heat flux from the flame to the inlet plane (where the burner is located) The distinctly different heat transfer characteristics of these two flames are immediately obvious. Even with the recycled flue gas, the oxy-gas flame is much hotter and consequently produces a higher radiative heat flux to surrounding surfaces. In Figure 4, the oxy-gas simulation was run with the soot radiation model turned off. These preliminary runs are to determine the parameters of interest for the V/UQ study.

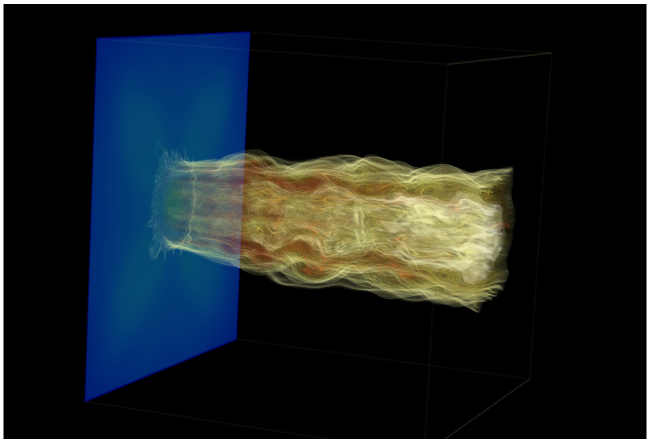


Figure 2: Volume-rendered image of air-gas flame in IFRF furnace fired with ENEL TEA-C burner showing heat flux to inlet plane (soot radiation turned on).

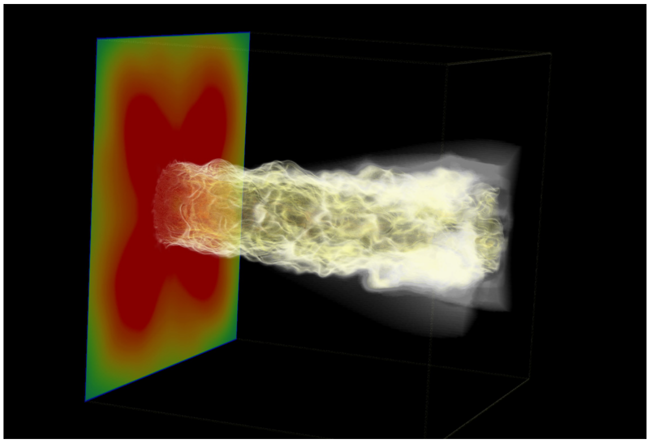


Figure 3: Volume-rendered image of oxy-gas flame in IFRF furnace fired with ENEL TEA-C burner showing heat flux to inlet plane (soot radiation turned on).

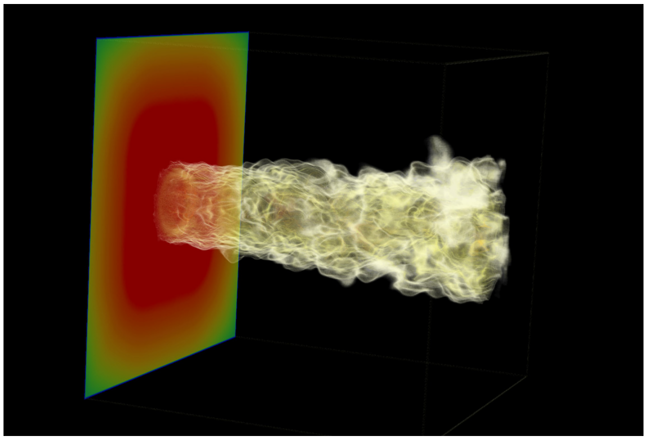


Figure 4: Volume-rendered image of oxy-gas flame in IFRF furnace fired with ENEL TEA-C burner showing heat flux to inlet plane (soot radiation turned off).

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

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

Using the commercial engineering process solver Star-CCM+, the Project Team is developing a high performance computing-based fluid and solid simulation of thermal processing of rubblized oil shale. In this quarter, team members have finalized their DEM simulation technique for creating individual pieces of shale, performed extended geometry simulations, as well as evaluated effects of boundary conditions on time evolution of the thermal profile inside the test capsule. Based on their preliminary results, they have identified improvements to the current design used by the project's industrial partner, Red Leaf Resources, that could favorably improve the thermal distribution inside the test capsule.

The Project Team also completed the milestone of implementing a correct geometry representation in Star-CCM+**.** Based on the two-pronged strategy described in the previous quarterly report, they have successfully implemented a simplified geometry representation of the trial experiment used by Red Leaf Resources in Star-CCM+ (see description below). However, team members will continue to evolve their DEM strategy to improve the geometry representation of the experimental domain in their simulations. Further achievements will be reported in the topical report.

Both Red Leaf Resources and Uintah Partners, a new player in oil shale production, have expressed the greatest interest in obtaining detailed information about the heat transfer to the shale. Thus, the Subtask 4.1 team has focused on answering this question and identifying parameters that have a first order effect on heat transfer.

Extended geometry results: In the previous quarterly report, the Project Team introduced a new, extended computational domain (see Figure 5) featuring two heating elements that more closely resembles a portion of the test bed geometry used by Red Leaf Resources to conduct their field experiment. It contains 470 pieces of shale, each created from 27 spherical elements instead of the 64 spherical elements used in previous simulations. This change reduces the computational cost of the DEM simulations and allows for geometry scale up without the memory usage issues described in the last quarterly report. The final computational mesh, including both the fluid and solid phases, contains 8.4 million polyhedral cells. For all simulations, the Project Team employed the laminar implicit solver for the fluid phase with a time step size of 0.2 seconds. The simulations ran on 612 processors, with 1 minute of simulation time corresponding to about 300 minutes of real time, highlighting the large computational cost associated with simulations involving heat transfer in both fluid and solid phases.

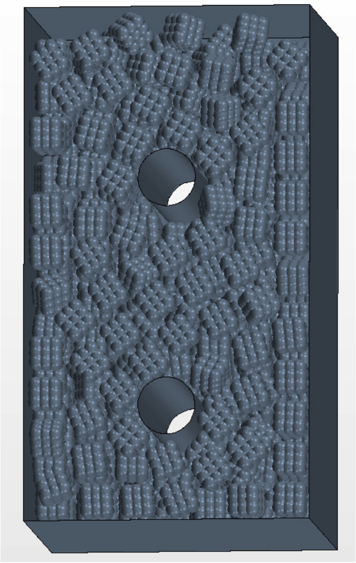


Figure 5: Extended computation domain used for fluid/solid simulation.

Figures 6, 7, and 8 show the coupled fluid/solid simulation results for the extended domain. Figures 6 and 7 show results after 418 time steps (83 seconds) and Figure 8 after 974 time steps (194 seconds). Buoyant velocities (Figure 6) approach 1.5 m/s in magnitude in the convective channels. The upward buoyant plume of hot air interacts with the geometry and mixes throughout the domain. The pieces of shale located in the direct pathway of the hot air convective current show the largest temperature change. Also of interest is the difference between the heating time of the fluid and of the solids. In the upper region of the domain, the temperature of the fluid increased by about 100 K from the initial stage, while the temperature of shale increased by only 2 to 4 K. This difference highlights the vastly different heating time scales for the fluid and solid regions.

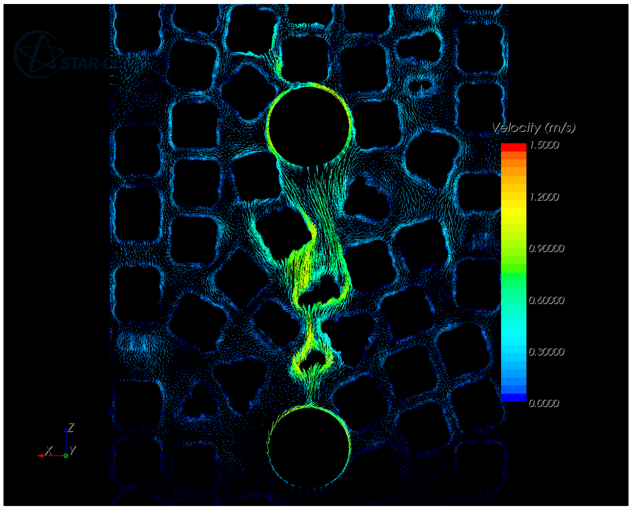


Figure 6: Fluid velocity profile in oil shale bed after 83 seconds.

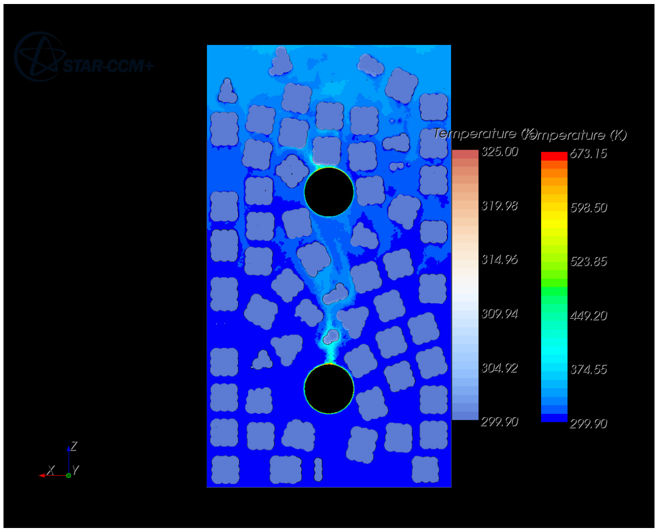


Figure 7: Fluid and solid temperature profiles in oil shale bed after 83 seconds.

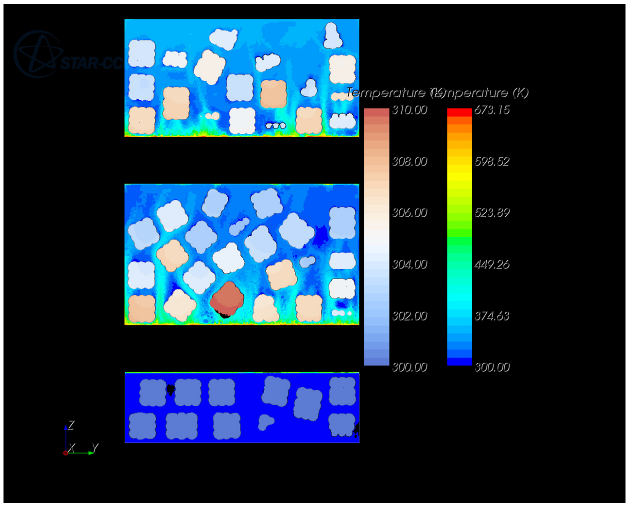


Figure 8: Fluid and solid temperature profiles in oil shale bed after 194 seconds.

Effects of boundary conditions on the thermal profile: Because of the large computational costs associated with extended-domain simulations of two phases, Subtask 4.1 researchers have conducted boundary condition sensitivity tests using the simplified domain shown in Figure 9 with a single fluid phase. The polyhedral mesh has 14 million elements in the fluid region alone. The implicit laminar solver is used with time step of 1 second. Three scenarios have been considered: 1) adiabatic (perfectly insulated) boundaries at the geometry edges and for the pieces of shale, 2) adiabatic boundaries at the geometry edges and constant temperature (300 K) boundary condition for the pieces of shale, and 3) constant temperature (300 K) boundaries for both the geometry edges and the pieces of shale. The constant 300 K boundaries for shale are based on the vastly different heating time scales for the fluid and solid regions. Because of the relatively short simulation times for these tests, the temperature increases in the pieces of shale are assumed to be negligible compared with temperature increase in the fluid region. This assumption reduces the computational cost by omitting the simulation of solid heat transfer. On the other hand, the constant 300 K temperature for the geometry edges represents a very poorly insulated system. Hence, these three scenarios span the extremes in boundary conditions expected for such a system in reality.

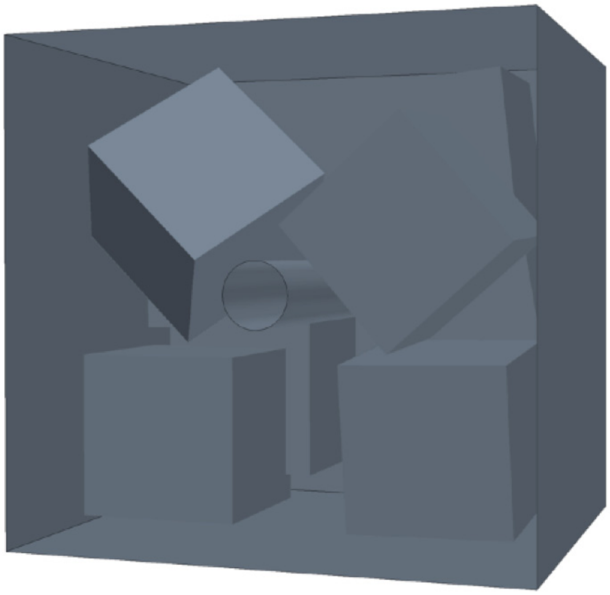


Figure 9: Simplified computational domain used in conjunction with fluid-only simulations to evaluate the effect of boundary conditions on the thermal profile inside the domain.

Figures 10, 11, and 12 show simulation results after 8861 seconds. The thermal profile inside the test bed is very sensitive to the boundary conditions. The greatest temperature increase is seen in the perfectly insulated system, Figure 10, while the smallest temperature increase is seen in the non-insulated system, Figure 12. The most realistic scenario with mixed boundary conditions (Figure 11) shows a temperature distribution in between the insulated and non-insulated systems. Therefore, it is very important 1) to insulate the experimental system extremely well to reduce heat losses, thus delivering more heat to the pieces of shale, and 2) to have an accurate description of experimental boundary conditions for a proper simulation-to-experiment comparison. Without knowing the exact experimental boundary conditions, it will be be difficult to obtain consistency between the simulated and the experimental temperature distribution inside the test bed.

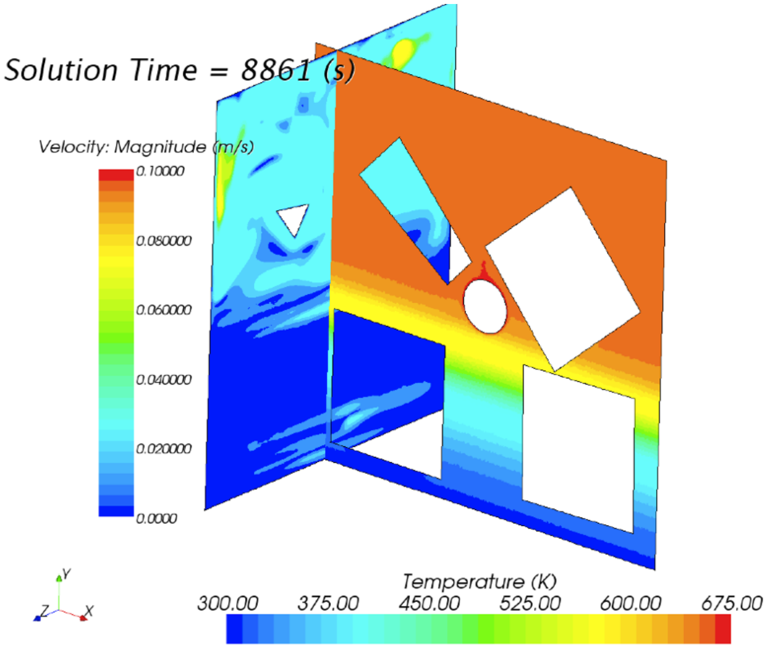


Figure 10: Temperature distribution inside a perfectly insulated domain.

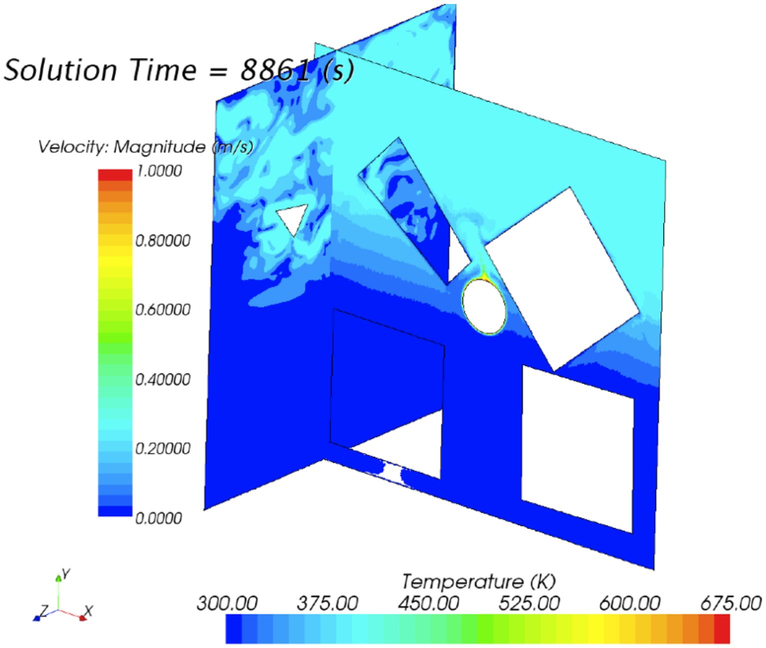


Figure 11: Temperature distribution inside a domain with perfectly insulated external boundaries and pieces of shale fixed at a constant temperature of 300 K.

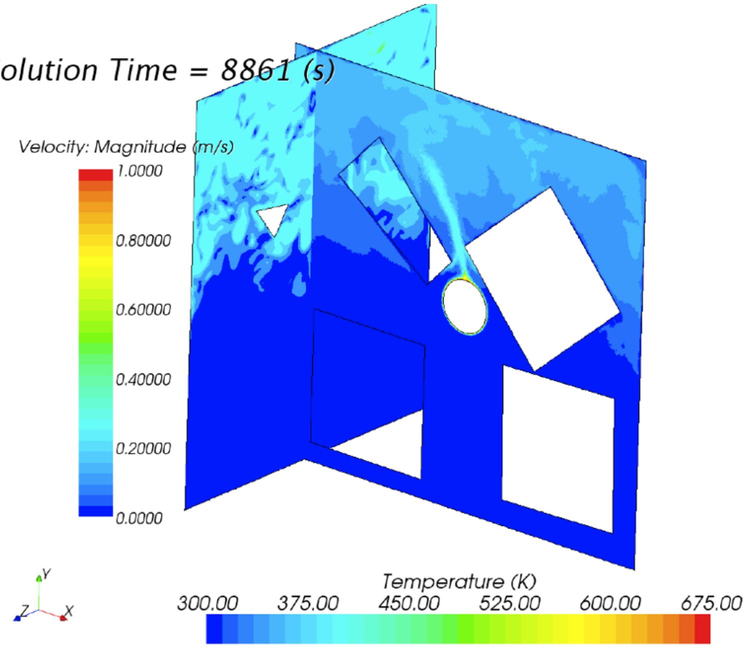
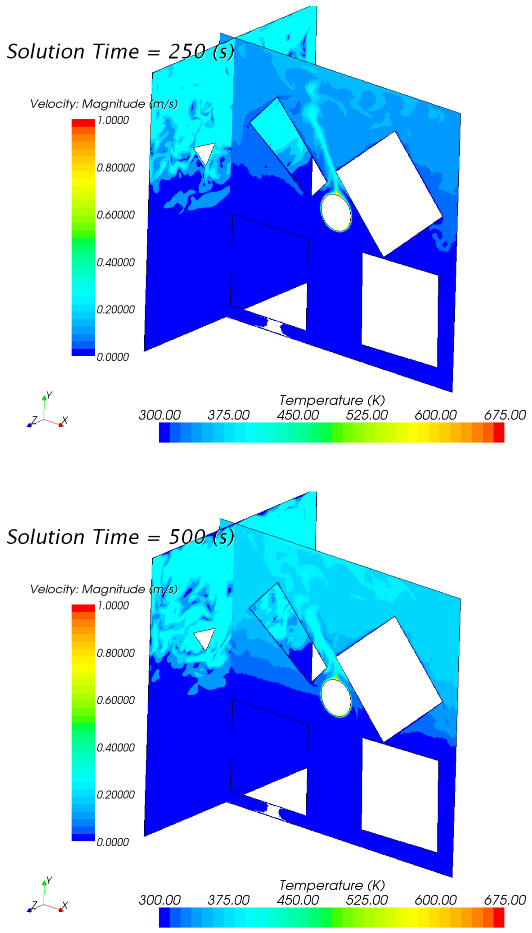


Figure 12: Temperature distribution inside a representative non-insulated domain.

Time evolution of the temperature profile: Subtask 4.1 researchers also used the simplified domain to better understand the time evolution of the temperature field inside the test bed. For this simulation, the same solver and time step as above were used along with the second boundary condition, e.g. perfectly insulated system boundaries and pieces of shale set at a constant temperature of 300 K. The results are shown in Figure 13. The greatest heating occurs in the first 1,000 seconds of the simulation, after which the overall heating rate inside the test bed decreases considerably. The initial heating is caused by the buoyant mixing of the hot air supplied by the heating element and the cool ambient air. As the air above the heating element increases in temperature, the buoyancy effect is considerably reduced. Most of the subsequent heat transfer occurs through conduction, greatly decreasing the overall heating rate. Based on these results, the best placement for the heating element would be as close to the bottom of the test bed as possible. Such a placement would allow for more effective buoyancy-driven mixing inside the test bed, thereby increasing the overall temperature inside the bed more rapidly.



t = 250 sec t = 500 sec

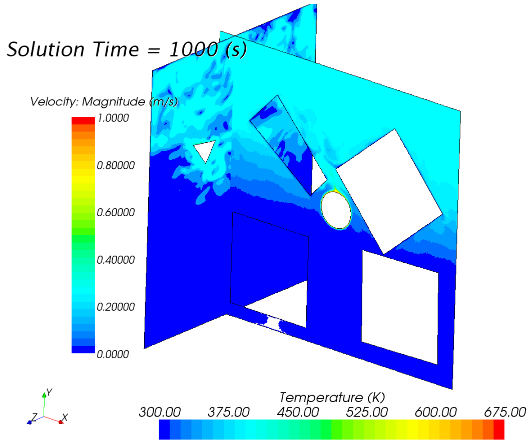


Figure 13: Time evolution of a thermal profile inside the simplified computational domain.

Subtask 4.2 - Basin-wide Characterization of Oil Shale Resource in Utah and Examination of In-situ Production Models (PI: Milind Deo)

Subtask 4.2 researchers completed several milestones and deliverables in this quarter. They synthesized data, finalized/completed the regional four-core cross section, and prepared, revised, and completed (with DOE approval) a final topical report accompanying the cross section. In addition, a paper entitled "Parameter Space Reduction and Sensitivity Analysis in Complex Thermal Subsurface Production Processes" was published in the journal *Energy and Fuels*.

Subtask 4.3 – Multiscale Thermal Processing of Oil Shale (PI: Milind Deo, Eric Eddings)

In this quarter, the Project Team completed a deliverable with the submission of the article entitled "Compositional and Kinetic Analysis of Oil Shale Pyrolysis Using TGA-MS " to the journal *Fuel*.

A comprehensive TGA study on Green River oil shale samples was reported earlier. In this report, the Project Team evaluated the effect of particle size and gas flow rate on TGA thermograms. A newer generation TGA-DSC was used in this work. The organic matter in the sample was approximately 10-12 weight %. Most of the experiments were conducted at a heating rate of 10°C/min. The raw sample was first pyrolyzed (in a nitrogen environment) to 1000°C and then, without opening the reactor chamber, the temperature was allowed to equilibrate at 400°C. The remaining material was combusted (in air) to temperatures of 600°C at the same heating rate.

Effect of particle size on pyrolysis decomposition process: Oil shale was crushed and screened to different mesh sizes. The samples were pyrolyzed and further combusted with the TGA-DSC unit as described. The flow rate of sweep gas was fixed at 50 ml/min. Other experimental conditions are summarized in Table 1 and the thermograms are shown in Figure 14. For clarity, the DSC signatures are not shown in the same figure. The thermograms are similar except for the 70 mesh particles, which means that heat and mass transfer effects can be avoided by using 100 mesh particles. Combustion environment thermograms show little or no coke on the samples.

Table 1. Pyrolysis (N_2) of different mesh size powdered oil shale (10-12 wt% organic).

N_2	Different size	Mass-mg	10C/min
1	+ 70 Mesh	8.57	1000C-600C
2	-70 +100m Mesh	8.9	1000C-600C
3	- 100 +140 Mesh	6.99	1000C-600C
4	-140+ 200Mesh	11.85	1000C-600C
5	- 200Mesh	7.64	1000C-600C

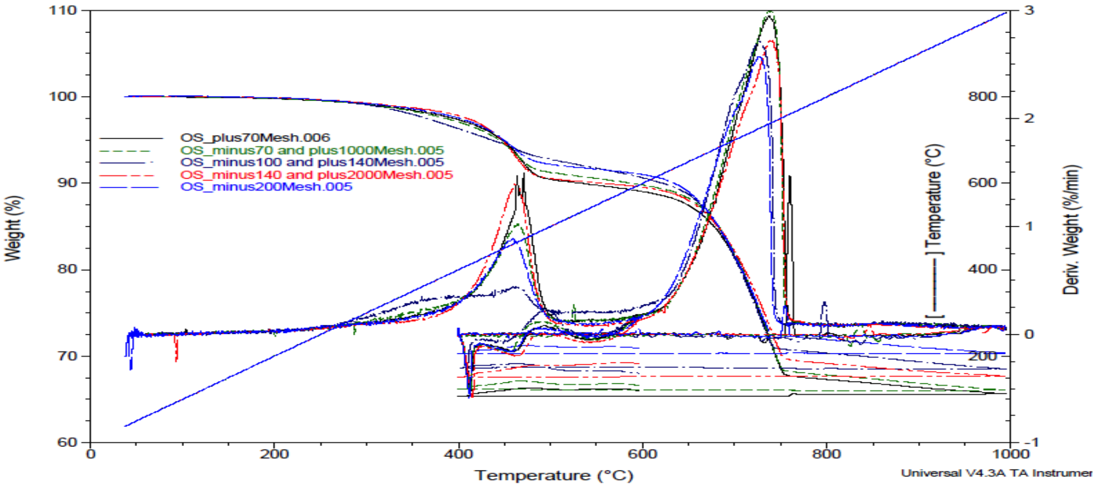


Figure 14: Pyrolysis (N_2) thermograms of different mesh size powdered oil shale (10-12 wt% organic).

Effect of sweep gas flow rate on the pyrolysis of oil shale samples (100-140 mesh): Oil shale crushed samples of -100+140 mesh size were pyrolyzed and further combusted under different sweep gas flow rates. Experimental conditions are shown in Table 2 and the data in Figure 15. At the highest flow rate (100 ml/min), the sharp peaks are indicative that heat transfer effects seen at low flow rates have been overcome.

Table 2. Pyrolysis (N_2) of powdered oil shale (10-12 wt% organic) with different sweep gas flow rates.

N_2	100-140mesh	Mass-mg	10C/min
1	0 ml/min	8.571	1000C-600C
2	25 ml/min	13.248	1000C-600C
3	50 ml/min	14.381	1000C-600C
4	100 ml/min	17.216	1000C-600C

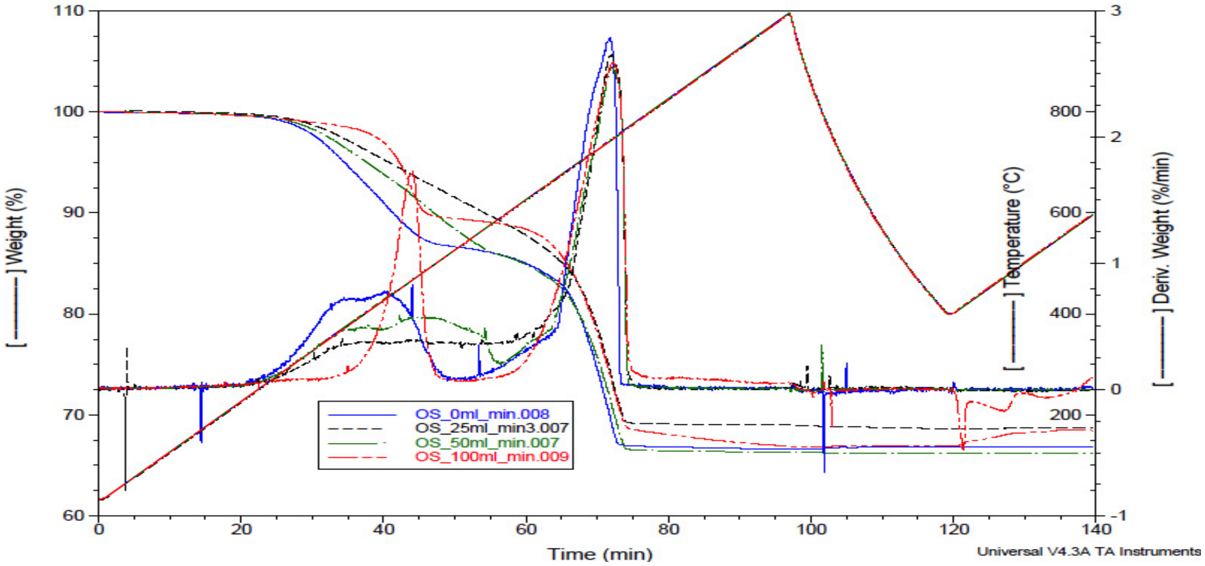


Figure 15: Pyrolysis (N_2) of powdered oil shale (10-12 wt% organic) with different sweep gas flow rates.

Multiscale modeling using COMSOL multiphysics module: When sufficient heat is supplied to oil shale, organic decomposition occurs to produce oil, gas and coke/char as primary products. A basic mathematical model for heat conduction and overall products formation (no diffusion and no convection) was developed in COMSOL with two-dimensional circular and rectangular geometries. The raw material (oil shale) is defined using physical properties (ρ, Cp , K) reported by Campbell et al. (1978) for 30 gal/ton grade oil shale. These physical properties are a function of the concentration of oil produced and are allowed to change as the reaction progresses. Details of the algorithms will be provided in later reports.

For the simulations, the grade of the oil shale is assumed to be 30 gal/ton, equivalent to an organic matter content of 18 wt%. Kerogen conversion to oil, gas, and coke is assumed to be 63 wt%, 24 wt% and 17 wt% respectively.

The governing equations are given below.

- *Heat transfer equation – Conduction and convection*

$$\rho\cdot Cp\frac{\partial T}{\partial t}+\nabla\left(-k\nabla T\right)=\cancelto{0}{Q}-\rho\cdot C\cancelto{0}{p}\cdot\vec{u}\nabla T$$

where ρ is overall density, C_p is heat capacity, k is thermal conductivity, and Q is the heat source (e.g. heat absorbed by reactions)

- *Mass transfer equation –Diffusion, convection and reaction*

$$\frac{\partial c_i}{\partial t} + \nabla\left(-\underset{0}{\cancel{D}}_{AB}\nabla c_i\right) = r_i - \vec{u}\underset{0}{\cancel{\nabla}}c_i$$

where c_i is the concentration of A (either c_O or c_G), DAB is the diffusion coefficient of A in B (= 10^{-15}, r_i is the reaction rate, and u is the velocity vector.

•Rate equations

Kerogen decomposition rate, r_k = - A*exp(E/RT)*C_k = [mol/(m^3·s)]

or, r_k = -K*C_k

where C_k is the concentration of kerogen. Constant values for the kinetic parameters assumed; the preexponential factor, A = 10^{-10}/s and activation energy, E = 200 kJ/mol.

Rate of [(- kerogen decomposition) = {(+f_1*oil) +(+f_2*gas) + (1-f_1-f_2)* coke formation]

- r_{oil} = K*Ck*f_1
- r_{gas} = K*Ck*f_2
- r_{coke} = K*Ck*(1-f_1-f_2)

where f_1 is the fractional conversion of kerogen to oil (63 wt%) and f_2 is the fractional conversion to gas (24 wt%).

Simulations were performed for various isothermal and nonisothermal cases. Figure 16 shows the temperature distribution profile along with changes in physical properties during pyrolysis with isothermal (500°C) boundary conditions for 1 minute duration in the 2D circular geometry (2 cm diameter). The non-isothermal simulations were performed at 10°C/min to 700°C and the concentration profiles of raw material and products at the circular geometry boundary are shown in Figure 17. These results are simply an illustration that a multiphysics module can be used to study the process. The next step is to validate the model using experimental results. The overall modeling scheme is shown in Figure 18.

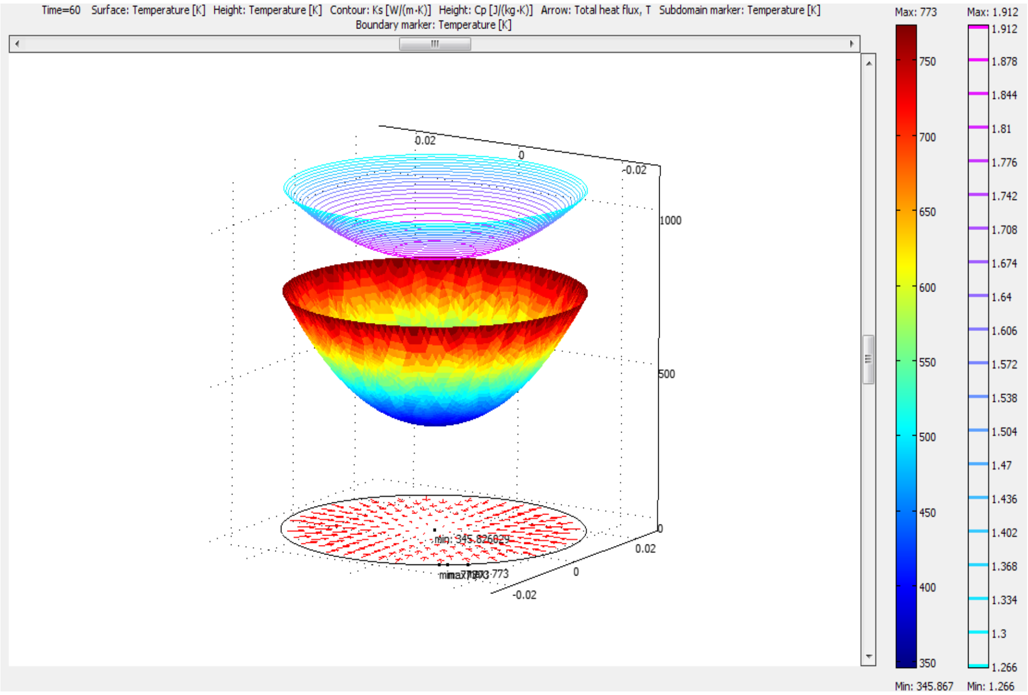


Figure 16: Simulation results from COMSOL multiphysics model with a simple reaction mechanism (overall product formation) for a material pyrolyzed at 500˚C for 1 minute. From top to bottom, grids show (1) thermal conductivity, (2) temperature, (3) heat flux.

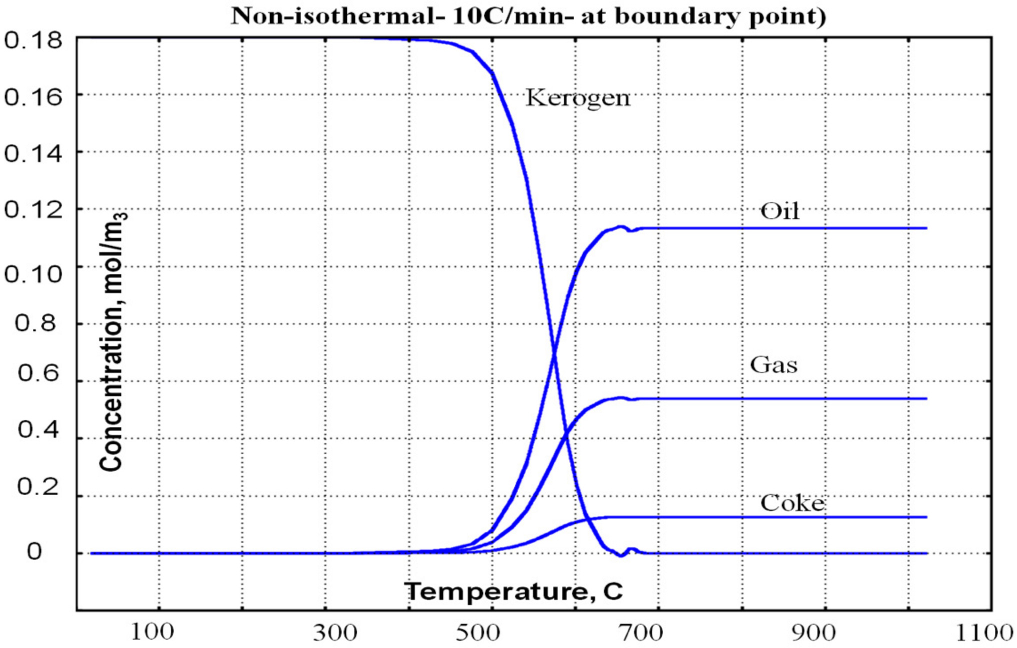


Figure 17: Concentration profiles of raw material and products at the boundary of the circular geometry from non-isothermal pyrolysis at 10˚C/min. The simulation was run for 100 minutes.

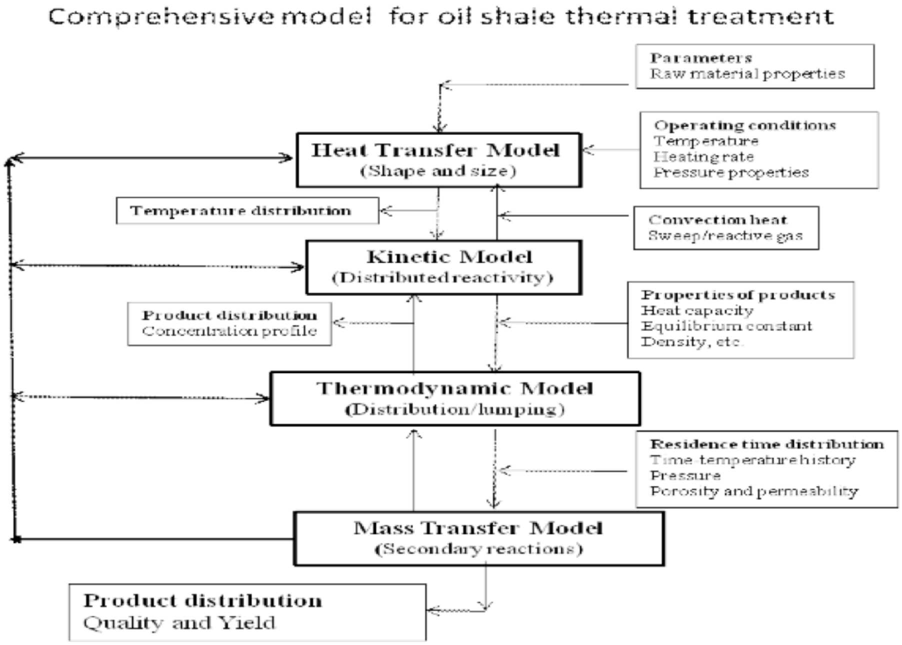


Figure 18: Mathematical modeling of oil shale pyrolysis process using COMSOL.

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

This subtask is associated with the Utah Geological Survey (UGS) project entitled "Water-related Issues Affecting Conventional Oil and Gas Recovery and Potential Oil-Shale Development in the Uinta Basin, Utah". The overall goals of this project are to (1) assess aquifers in the Uinta Basin to determine where saline water (produced along with conventional petroleum development) can be disposed without harming freshwater resources, and (2) to study how oil shale development would affect water quality in the Bird's Nest aquifer where there is currently significant water disposal. In this quarter, the Project Team reports experimental results for both hydrous and non-hydrous pyrolysis experiments. In addition, the milestone to determine compositional impact of soluble pyrolysis products on a reservoir scale was completed. The title slide from a presentation on this work is included in Appendix C of this report. The presentation will be sent to the Program Manager as a separate document.

Hydrous pyrolysis: These experiments were performed with oil shale cores and deionized water (Figure 19). Oil shale cores (3/4" diameter) from the Green River formation (Mahogany zone) were used for the hydrous pyrolysis experiments. The duration of the experiments was 72 hours. The reactor assembly was then cooled down and the liquid and gas samples were collected for analysis.

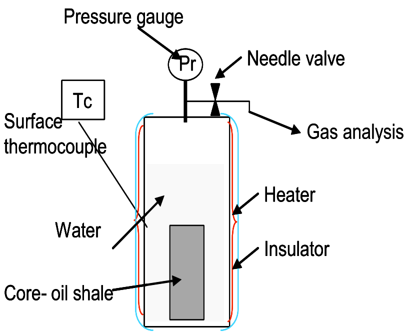


Figure 19: Experimental setup for hydrous pyrolysis experiments.

First, three experiments were set up for hydrous pyrolysis at temperatures of 300˚C, 400˚C and 500˚C with the aim of performing isothermal experiments for a duration of three days. The pressure readings for all three runs are shown Figure 20. The rapid increase in pressure for the experiment at 500˚C led to the discontinuation of that experiment. The experiment at 400˚C was run at 350˚C after 25 minutes.

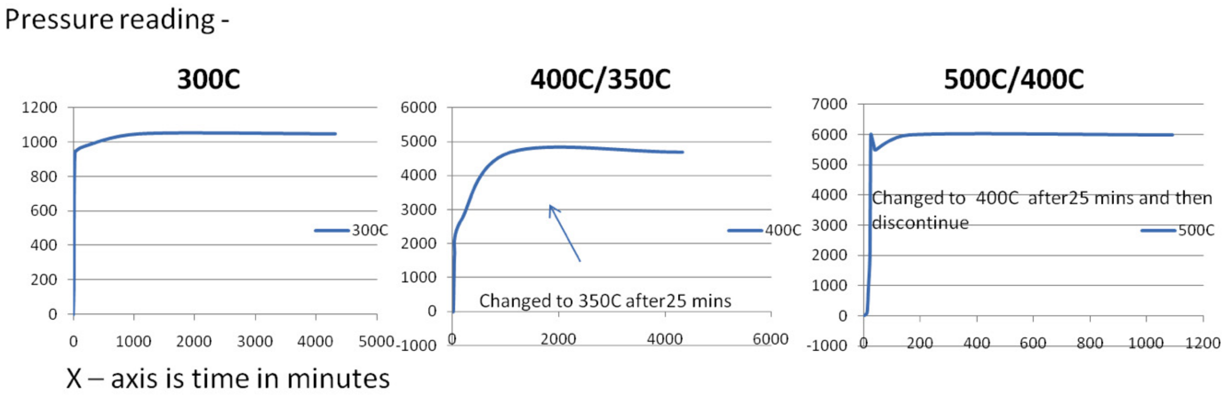


Figure 20: Pressure increase during batch hydrous pyrolysis experiments at different temperatures.

Figure 21 shows gas chromatograms of the gas and liquid (water and oil) samples and the TGA-DSC thermograms on spent shales. No significant hydrocarbon compounds were detected in the water phase sample chromatograms for either the 300˚C or the 350˚C experiments. The analysis of the gas sample from the 350˚C experiment shows a distribution of light hydrocarbon gases (some heavier than C7 carbon). TGA-DSC data reveal that there was a significant amount of unreacted organic (8% of spent shale) remaining on the solid residues from the 300˚C experiment while the 350˚C spent shale contained a large amount of water (6 wt% in spent shale). None of the samples show a significant amount of coke.

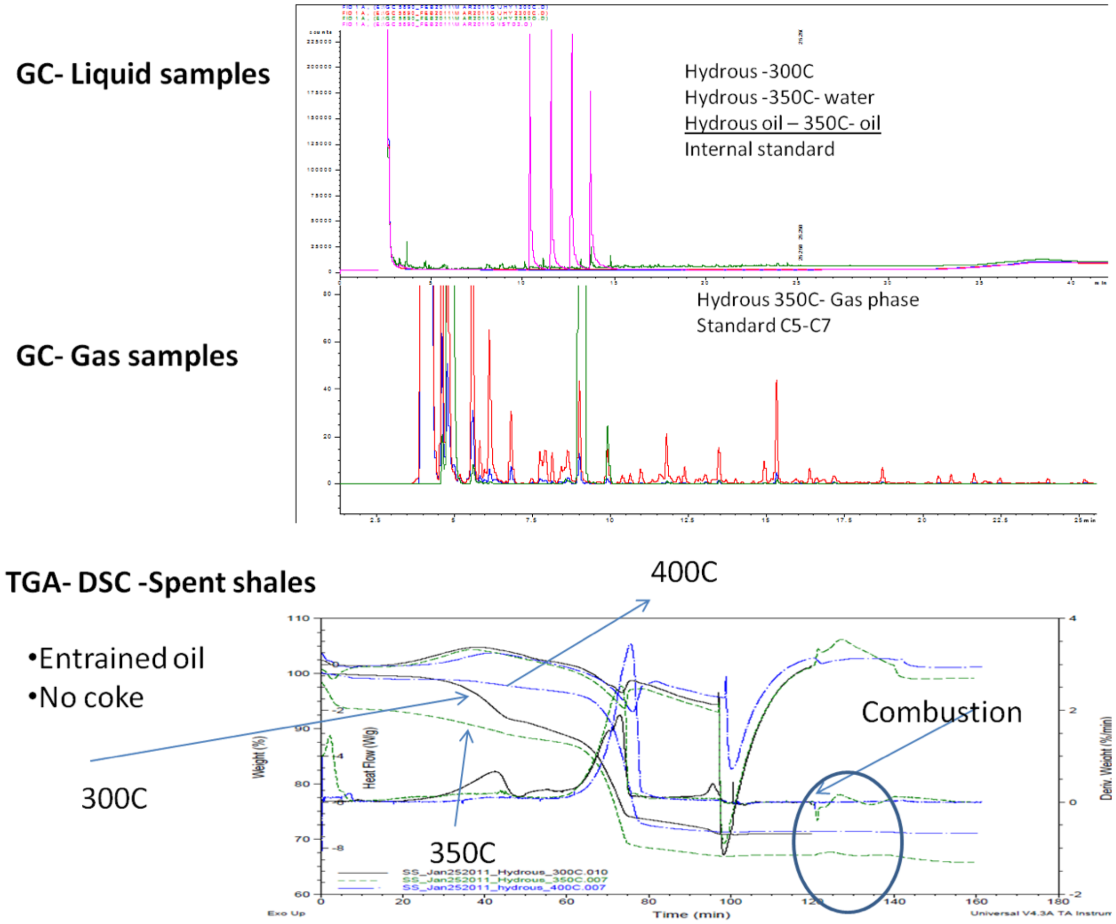


Figure 21: Analyses of hydrous pyrolysis products (gas, liquid and spent shale).

Non-hydrous pyrolysis - When water is associated with the organic matter in shale, the pyrolysis process has the potential of producing water. There is little water associated with the core samples from the Mahogany zone of the Green River formation. Hence, pyrolysis of two large core samples (2.5” in diameter) was required to produce a sufficient amount of water for analysis. The non-hydrous experiments (N_2 was the sweep gas at a flow rate of 100 ml/min) were performed for 48 hrs at 350˚C under ambient pressure and at 500˚C under 500 psi pressure. The water produced during pyrolysis was collected and analyses were performed by American West Analytical Laboratory (AWAL) located in Salt Lake City, Utah.

To perform the analyses on the water phase sample, different laboratory grade surrogates were used.

1. Total organic carbon (TOC) in the water sample (A5310B).
2. Oil and Grease (OnG) in the water sample- (Method E1664A).
3. Volatile organic in the water using GCMS (Gas Chromatography Mass Spectrometry - (Method -SW-846 8260C/5030C)
4. Semi volatile organic in water using GCMS- (Method-SW-846 8270D/3510C)

Five samples from batch hydrous pyrolysis and non-hydrous continuous flow pyrolysis (shown below) were analyzed at AWAL, including four water phase and one oil phase sample.

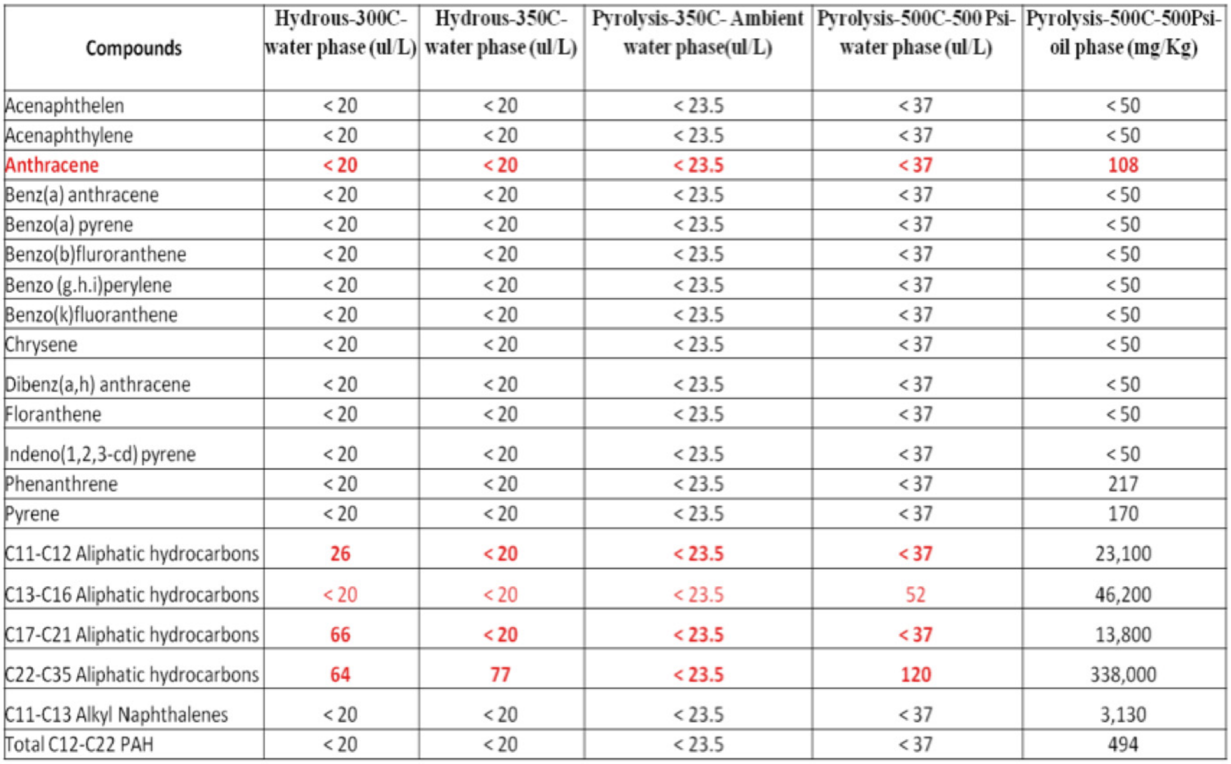
1. Hydrous-1- Batch -300˚C-72hrs -water phase
2. Hydrous-2- Batch- 350˚C- 72hrs - water phase
3. Pyrolysis-350˚C-ambient Psi-2.5"- water phase (Data on this sample was reported in an earlier quarterly report).
4. Pyrolysis-500˚C-500 Psi-2.5"- water phase
5. Pyrolysis-500˚C-500Psi-2.5"- oil phase

The gas chromatography/mass spectrometry (GCMS) data obtained for volatile and semi-volatile hydrocarbons are compared in Tables 3 and 4. The chromatograms show that most of the targeted compounds, including the potential aromatics, were below the detection limit of the instrument (method) used. The C_7-C_{35} aliphatic hydrocarbons are present in all the water phase samples and their amount increased with increase in pyrolysis temperature. The oil phase sample shows a wide range of hydrocarbon species (including the aromatics, PAH); these species have the potential to be sources of contamination if in contact with water for long duration. The GCMS analyses of all these samples also revealed some untargeted compounds like acid and alcohol groups.

Table 3. GCMS results for targeted volatile components.

Compounds	Hydrous-300C-water phase (ul/L)	Hydrous-350C-water phase (ul/L)	Pyrolysis-350C-water phase(ul/L	Pyrolysis-500C-500 Psi-water phase (ul/L)	Pyrolysis-500C-500Psi-oilr phase (ug/Kg)
Benzene	< 200	< 1,000	< 2,000	< 2,000	943,000
Ethylbenzene	< 200	< 1,000	< 2,000	< 2,000	1,730,000
Methyl-tert-butyl ether	< 200	< 1,000	< 2,000	< 2,000	< 50,000
Naphthalene	< 200	< 1,000	< 2,000	< 2,000	766,000
Toluene	< 200	< 1,000	< 2,000	< 2,000	5,030,000
Xylenes,Total	< 200	< 1,000	< 2,000	< 2,000	8,500,000
C6 Apliphatic hydrocarbons	< 200	< 1,000	< 20,000	< 20,000	4,540,000
C7&C8 Aliphatic hydrocarbons	15,700	42,100	< 20,000	< 20,000	34,500,000
C9&C10 Aliphatic hydrocarbons	< 2,000	< 10,000	< 20,000	< 20,000	23,300,000
C9&C10 Alkyl Benzenes	< 2,000	< 10,000	< 20,000	< 20,000	6,540,000

Table 4. GCMS results for targeted semi-volatile components.



Compounds	Hydrous-300C-water phase (ul/L)	Hydrous-350C-water phase (ul/L)	Pyrolysis-350C- Ambient water phase(ul/L)	Pyrolysis-500C-500 Psi-water phase (ul/L)	Pyrolysis-500C-500Psi-oil phase (mg/Kg)
Acenaphthelen	< 20	< 20	< 23.5	< 37	< 50
Acenaphthylene	< 20	< 20	< 23.5	< 37	< 50
Anthracene	< 20	< 20	< 23.5	< 37	108
Benz(a) anthracene	< 20	< 20	< 23.5	< 37	< 50
Benzo(a) pyrene	< 20	< 20	< 23.5	< 37	< 50
Benzo(b)fluroranthene	< 20	< 20	< 23.5	< 37	< 50
Benzo (g.h.i)perylene	< 20	< 20	< 23.5	< 37	< 50
Benzo(k)fluoranthene	< 20	< 20	< 23.5	< 37	< 50
Chrysene	< 20	< 20	< 23.5	< 37	< 50
Dibenz(a,h) anthracene	< 20	< 20	< 23.5	< 37	< 50
Floranthene	< 20	< 20	< 23.5	< 37	< 50
Indeno(1,2,3-cd) pyrene	< 20	< 20	< 23.5	< 37	< 50
Phenanthrene	< 20	< 20	< 23.5	< 37	217
Pyrene	< 20	< 20	< 23.5	< 37	170
C11-C12 Aliphatic hydrocarbons	26	< 20	< 23.5	< 37	23,100
C13-C16 Aliphatic hydrocarbons	< 20	< 20	< 23.5	52	46,200
C17-C21 Aliphatic hydrocarbons	66	< 20	< 23.5	< 37	13,800
C22-C35 Aliphatic hydrocarbons	64	77	< 23.5	120	338,000
C11-C13 Alkyl Naphthalenes	< 20	< 20	< 23.5	< 37	3,130
Total C12-C22 PAH	< 20	< 20	< 23.5	< 37	494

Subtask 4.5 - Pore Scale Analysis of Oil Shale/Sands Pyrolysis (PI: Jan Miller, Chen-Luh Lin)

Research on pore scale transport processes in the pyrolysis of oil sand and oil shale involves multi-scale, 3D X-ray micro computed tomography (XMT) analysis coupled with Lattice Boltzmann (LB) simulation. In the quarter, the Project Team completed a topical report that was approved by DOE.

Future research will identify critical fundamental factors of pore geometry and structure which limit recovery of hydrocarbons from oil sands and oil shale. This research will include:

- Analysis of new, fresh oil shale core and comparison with the initial oil shale samples
- Calibration for phase identification with results from QEM/SCAN.
- Directional (anisotropic) permeability of the new oil shale samples after pyrolysis reactions at different temperatures based on pore network structure by XMT analysis coupled with LB simulation.
- Permeability of the reacted core after pyrolysis reactions under different loading conditions.

Subtask 4.6 - Kerogen/Asphaltene/Mineral Matrix: Structure and Interactions (PI: Julio Facelli, Ronald Pugmire)

The Project Team submitted a topical report on the results from 3D modeling of kerogen and asphaltenes. As part of that report, team members calculated the NMR data for previously modeled kerogen and simulated the pyrolysis of the previously modeled Campana asphaltenes proposed by Siskin et al (2006) and discussed in the last quarterly report. In addition, the first trip to the Advanced Photon Source at Argonne National Labs was made and data (atomic pairwise distribution function and small angle X-ray scattering measurements) were obtained on oil shale samples from the Skyline 16 core as well as on a kerogen sample isolated from one section of this core. These experimental data will be used to evaluate the 3D kerogen structure based on the Siskin model obtained by previous computational efforts of the Project Team.

For the NMR calculation of kerogen, Subtask 4.6 researchers took the previously modeled single unit of kerogen and implemented the density functional theory with functional PBE0 using the 4-31G basis set. The calculated spectrum is shown in Figure 22. For comparison, the preliminary experimental ^{13}C NMR spectrum obtained on the kerogen isolated from a section of the Skyline 16 core is shown in Figure 23.

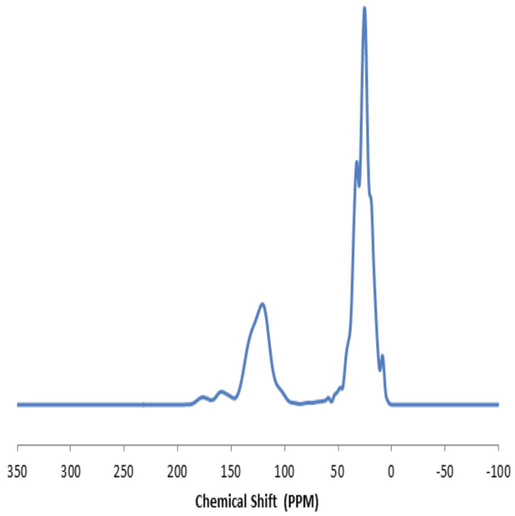


Figure 22: Calculated ^{13}C NMR spectrum for kerogen based on single unit of kerogen model.

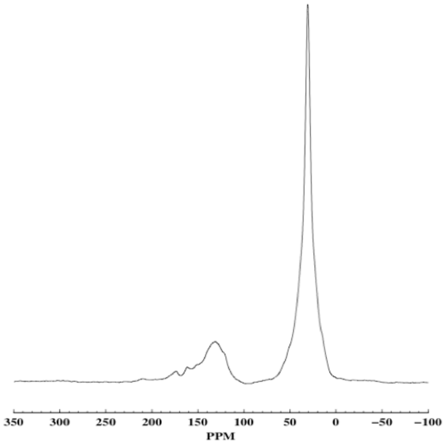


Figure 23: Experimental ^{13}C NMR spectrum from Skyline 16 core sample in Mahogany zone at depth of 462-463 feet.

Initially, the implementation of ReaxFF in the molecular dynamics simulation program LAMMPS was explored as a way to model pyrolysis of oil shale and sands. However, simulations with the stand alone ReaxFF program showed that it was a better choice. Using this program, the Project Team has modeled the pyrolysis process under constant number of atoms, volume and temperature (NVT) conditions for the 3D Campana asphaltene structure as well as its three different stacks. The results for the pyrolysis of the single Campana asphaltene at different temperatures are shown in Figure 24. From this figure, it is clear that the number of the product molecules increases with increasing temperature and with time evolution at a particular temperature. The results for the three different stacks are presented in Figures 25, 26, and 27. These results show a similar trend to the single Campana asphaltene unit: an increasing number of product molecules with increasing temperature.

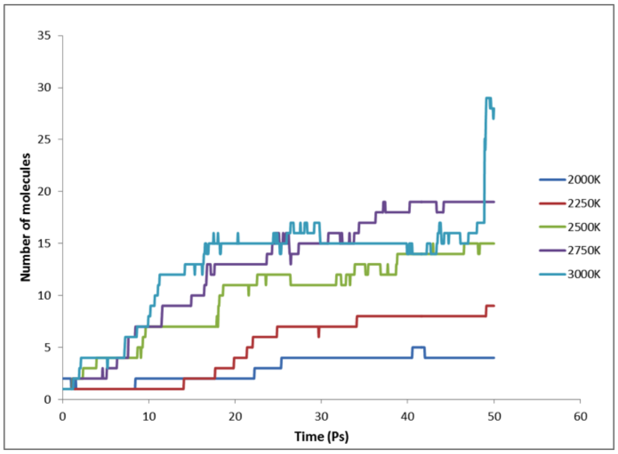


Figure 24: Results of NVT-MD simulation of a single Campana asphaltene unit at different temperatures.

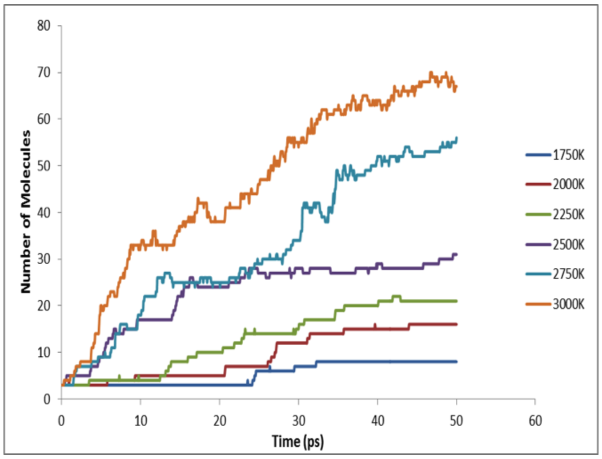


Figure 25: Results of NVT-MD simulation of parallel stack of three Campana asphaltene units at different temperatures.

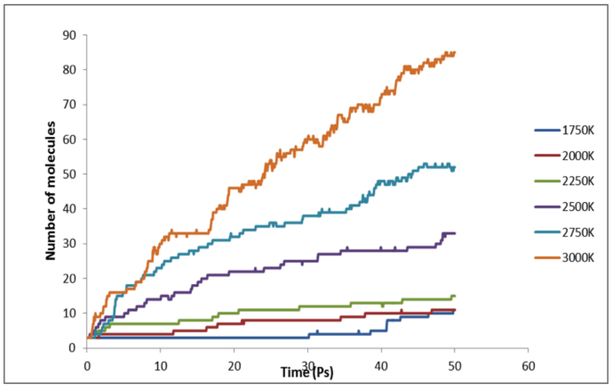


Figure 26: Results of NVT-MD simulation of anti-parallel stack of three Campana asphaltene units at different temperatures.

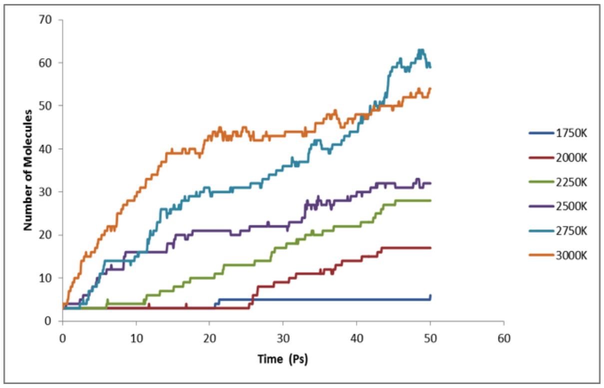


Figure 27: Results of NVT-MD simulation of inverted stack of three Campana asphaltene units at different temperatures.

Recently, the force field for the sulfur became available, allowing for similar simulations for the other five asphaltenes and the kerogen.

Subtask 4.7 - Geomechanical reservoir state (PI: John McLennan)

During this quarter, Subtask 4.7 researchers created fabrication drawings for the triaxial pressure vessel shown in Figure 28. In addition, third party components were ordered. The preliminary drawings were submitted to an ASME-certified design firm to ensure pressure ratings can be met.

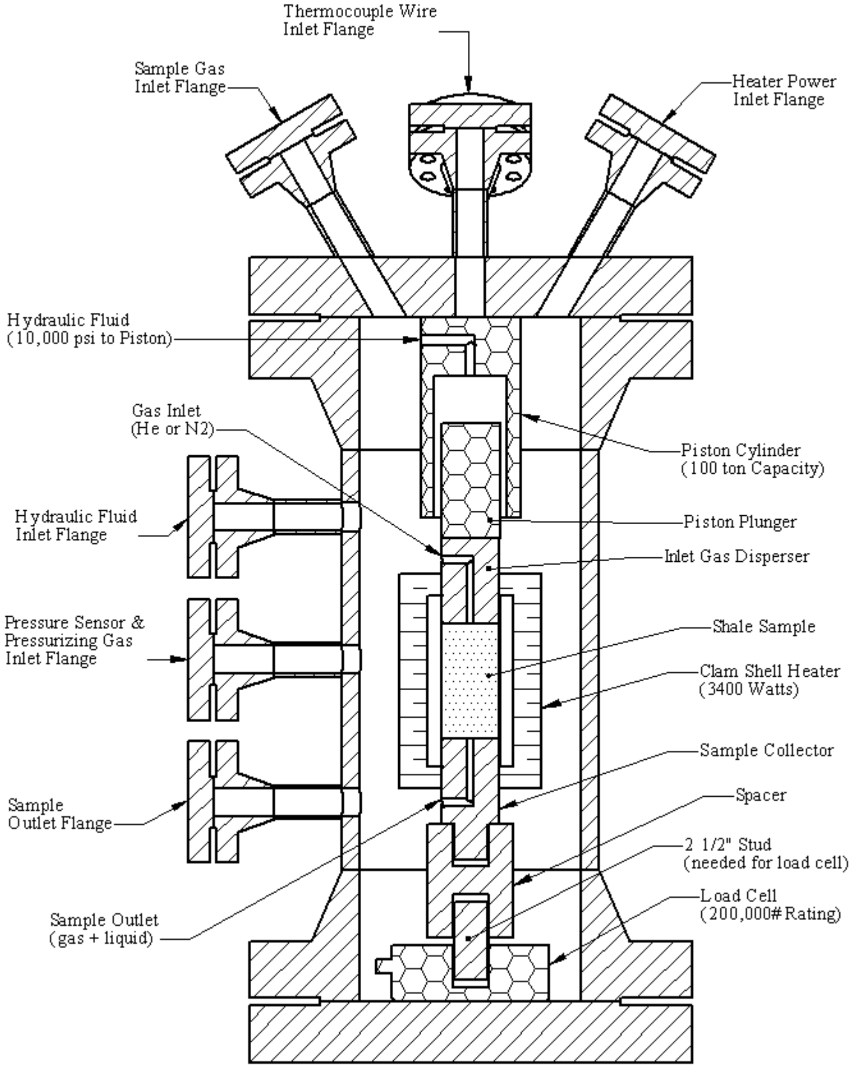


Figure 28: Large diameter pressure vessel with access and viewing flanges, internal triaxial vessel, clam shell heaters, and inlet and outlet ports for fluid and instrumentation. Maximum diameter of shale sample is 4-inches (shown to scale).

Task 5.0 - Environmental, Legal, Economic and Policy Framework

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

The Project Team, in conjunction with the University's Digitally Integrated Geographic Information Technologies Lab (DIGIT Lab), obtained public land inventory and management data from the BLM and categorized land management requirements in terms of the direct and cumulative level of constraint they pose for ground-disturbing activities on federal public lands. The DIGIT Lab also obtained energy resource information from the Utah Geological Survey in order to refine prior assessments of resource ownership and control. The DIGIT Lab has begun overlaying the constraints analysis on the resource inventory to evaluate constraints to oil shale and tar sands access. Researchers also began reviewing the Department of the Interior's revised policy regarding management of wilderness quality public and began drafting an explanation of the policy and challenges to its implementation. The DIGIT Lab is mapping federal public lands within Utah that have been inventoried as possessing wilderness characteristics, enabling a quantitative assessment of the effect of the newly issued Interior policy.

Subtask 5.1 researchers also reviewed scholarly publications regarding the prerequisites for effective resource management collaboration, focusing on scholarship specific to natural resource and public lands management. This research provides the analytical framework for reviewing cross-jurisdictional management case studies. Research indicates that communities' social and economic conditions as judged against the conditions of peer communities play an important role in determining community acceptance of conservation oriented land and resource management programs. Accordingly, researchers have begun compiling data on measures of community well being (e.g., access to health care, educational attainment, home ownership, income, crime, etc.) for Uintah County, the State of Utah, and the United States. This data will be used to develop a community profile and improve understanding of the perspective from which energy production and public land dependent communities view public land management efforts.

Lastly, Subtask 5.1 researchers began analyzing potential natural resource management case studies, focusing on two related categories of projects that have been undertaken within Utah: (1) efforts to consolidate land ownership through land exchange proposals, and (2) efforts to legislatively or administratively protect federal public lands. Researchers have identified six large land exchange proposals initiated during the last thirty years and have begun researching project specifics. Additionally, researchers have identified four substantively different efforts to protect federal public lands in Utah (establishment of the Grand Staircase-Escalante National Monument, the Cedar Mountain Wilderness Area designation, the Washington County Lands Bill, and the Red Rock Wilderness Bill) and have begun evaluating these four projects in the context of the analytical framework outlined above.

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

The Project Team conducted research regarding the historic development of and recent updates to legal requirements applicable to surface water management, groundwater management, and conjunctive water management. The project team also researched conjunctive surface and groundwater management efforts in the Salt Lake Valley and in southwestern Utah. The project team tracked state legislation affecting local district's authority to initiate and fund conjunctive management projects and met with water law experts, including attorneys from the Office of the Utah Attorney General and local water managers, to obtain information regarding conjunctive water resource project implementation. The project team continued drafting an article addressing conjunctive surface and groundwater management within Utah. The Idaho Law Review has accepted this article for publication, with publication anticipated later in 2011.

6.0 – Economic and Policy Assessment of Domestic Unconventional Fuels Industry

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

Subtask 6.1 researchers continued to refine process models for in situ production scenarios associated with heavy oil, oil sands, and oil shale and to draft/refine sections of the Market Assessment. Due to the considerable scope of the scenarios in the assessment and the wide range in uncertainty of the inputs, the emphasis this quarter was on performing sensitivity analyses on inputs with high uncertainty and strong impacts on production costs. This work is reported in the sections that are being drafted

Subtask 6.2 - Policy analysis of the Canadian oil sands experience (PI: Kirsten Uchitel)
During this quarter, Subtask 6.2 researchers completed research and analysis related to taxes and royalties levied on oil sands production, as well as downstream and marketing challenges facing oil sands development. Specifically, Subtask 6.2 researchers (1) examined the economic basis of mineral taxation, including the notion of "economic rent," which has played a central role in the theory and practice of mineral taxation policy, (2) reviewed the historical and current tax and royalty policies ("fiscal system") applying to the Alberta oil sands, and (3) reviewed fiscal systems applying to conventional onshore oil production in the U.S. Researchers also completed analysis and writing of their economic research findings and applied those research findings to the issues addressed in the Oil Sands Topical Report. Researchers specifically addressed the relevance for oil sands development of two general research findings: (1) if the primary goal of mineral taxation policy is to encourage development, then the standard U.S. fiscal system applying to conventional onshore production may be a poor choice for unconventional production as the standard U.S. fiscal system is largely based on the gross revenues from extracting oil from a deposit, rather than the rent of the deposit; and (2) the low rent of unconventional resources such as oil sands and oil shale does not imply that they should be taxed delicately (e.g. according to rent) as policymakers may decide that the negative environmental or sociological side-effects are severe enough that purposeful, active discouragement of such projects is warranted.

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

The Project Team prepared a draft of the Market Assessment report. Part one of that draft was sent to reviewers just after the end of this quarter. Work continues on the second part. The list of reviewers includes Alan Burnham (American Shale Oil), Gary Aho (Sage Geotech), Laura Nelson (Red Leaf Resources), Vince Memmott (Uintah Partners), Julia Haggerty (Headwaters Economics), Robert Vagnetti (DOE/NETL), Olayinka Ogunsola (DOE), Glen Snarr (Earth Energy Resources), Michael Vanden Berg (Utah Geological Survey), and Andrew Wolfsberg (Los Alamos National Laboratory).

CONCLUSIONS

The Clean and Secure Energy from Domestic Oil Shale and Oil Sands Resources program is wrapping up milestones and deliverables for FY2009 in preparation for moving on to FY2010 work. This report marks the completion of Phase I for several of the projects and the initiation of a new project (Subtask 4.7). In the next quarterly report, all new projects will be phased in and the project end date will change to September 2013.

COST STATUS

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

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

Baseline Reporting Quarter - PHASE II	Yr. 2				Yr. 3							
	Q7		Q8		Q9		Q10		Q11		Q12	
	04/01/11 - 06/30/11		07/01/11 - 09/30/11		10/01/11 - 12/31/11		01/1/12 - 03/31/12		04/01/12 - 06/30/12		07/01/12 - 09/30/12	
	Q7	**Total**	Q8	**Total**	Q9	**Total**	Q10	**Total**	Q11	**Total**	Q12	**Total**
Baseline Cost Plan												
Federal Share	712,385	**3,773,026**	627,423	**4,400,449**	147,451	**4,547,900**	147,451	**4,695,351**	147,451	**4,842,802**	245,447	**5,088,249**
Non-Federal Share	178,100	**943,509**	156,854	**1,100,363**	36,863	**1,137,226**	36,863	**1,174,089**	36,863	**1,210,952**	58,906	**1,269,858**
Total Planned	890,485	**4,716,535**	784,277	**5,500,812**	184,314	**5,685,126**	184,314	**5,869,440**	184,314	**6,053,754**	304,353	**6,358,107**
Actual Incurred Cost												
Federal Share		**2,629,270**		**2,629,270**		**2,629,270**		**2,629,270**		**2,629,270**		**2,629,270**
Non-Federal Share		**650,635**		**650,635**		**650,635**		**650,635**		**650,635**		**650,635**
Total Incurred Costs		**3,279,905**		**3,279,905**		**3,279,905**		**3,279,905**		**3,279,905**		**3,279,905**
Variance												
Federal Share		**1,143,756**		**1,771,179**		**1,918,630**		**2,066,081**		**2,213,532**		**2,458,979**
Non-Federal Share		**292,874**		**449,728**		**486,591**		**523,454**		**560,317**		**619,223**
Total Variance		**1,436,630**		**2,220,907**		**2,405,221**		**2,589,535**		**2,773,849**		**3,078,202**

Baseline Reporting Quarter - PHASE II	Yr. 4											
	Q13		Q14		Q15		Q16					
	10/01/12 - 12/31/12		01/01/13 - 03/31/13		04/01/13 - 06/30/13		07/01/13 - 09/30/13					
	Q13	**Total**	Q14	**Total**	Q15	**Total**	Q16	**Total**		**Total**		**Total**
Baseline Cost Plan												
Federal Share	146,824	**5,235,073**	146,824	**5,381,897**	146,824	**5,528,721**	133,794	**5,662,515**				
Non-Federal Share	36,705	**1,306,563**	36,705	**1,343,268**	36,705	**1,379,973**	35,906	**1,415,879**				
Total Planned	183,529	**6,541,636**	183,529	**6,725,165**	183,529	**6,908,694**	169,700	**7,078,394**				
Actual Incurred Cost												
Federal Share		**5,088,249**		**5,088,249**		**5,088,249**		**5,088,249**				
Non-Federal Share		**1,269,858**		**1,269,858**		**1,269,858**		**1,269,858**				
Total Incurred Costs		**6,358,107**		**6,358,107**		**6,358,107**		**6,358,107**				
Variance												
Federal Share		**146,824**		**293,648**		**440,472**		**574,266**				
Non-Federal Share		**36,705**		**73,410**		**110,115**		**146,021**				
Total Variance		**183,529**		**367,058**		**550,587**		**720,287**				

MILESTONE STATUS

ID	Title/Description	Planned Completion Date	Actual Completion Date	Milestone Status
1.0	Project Management			
	Project management plan	Nov-09	Dec-09	
	Briefings & reports	Mar-11		Ongoing
2.0	Technology Transfer and Outreach			
	Upload geodatabase of water information to map	Mar-10	Mar-10	Reported in Q1 2010 report
	Hold project review meeting in the form of presentations/poster session at ICSE-sponsored unconventional fuels conference	May-10	Apr-10	Reported in Q2 2010 report
	Complete addition of research materials from each task listed below to online digital repository	May-10		200 documents are entered, but collection does not include materials from every task
	Implement interactive map usage tracking or determine that it is not feasible	Jun-10	Jun-10	Reported in Q2 2010 report
	Advisory board meeting	Jun-10	Apr-10	Reported in Q2 2010 report
	Deploy updated web mapping software	Jul-10	Sep-10	Deployment cancelled due to departure of employee
	Upgrade Dspace platform for digital repository	Aug-10	Aug-10	Reported in Q3 2010 report
	Standardize and improve map attribute information	Jan-11		Cancelled due to departure of employee
	Completion of student research experiences	Mar-11		No students participated in research over the summer, so this milestone will not be met
	Tech transfer workshop, conference, & forums	Mar-11	Mar-11	
	Hold final project review meeting in format determined jointly by DOE/NETL and ICSE	Mar-11	Mar-11	

ID	Title/Description	Planned Completion Date	Actual Completion Date	Milestone Status
3.0	Clean Oil Shale & Oil Sands Utilization with CO2 Management			
3.1	Macroscale CO2 analysis			
	Identify & collect experimental, literature, & simulation data on GHG emissions from process heaters	Mar-10	Mar-10	Reported in Q2 2010 report
	Identify or develop appropriate tool for predicting life-cycle GHG emissions from a given technology	Sep-10	Nov-10	Reported in this quarterly report
3.2	Flameless oxy-gas process heaters for efficient CO2 capture			
	Preliminary report detailing results of skeletal validation/uncertainty quantification analysis of oxy-gas combustion system	Nov-10		Delayed due to coding issues
4.0	Liquid Fuel Production by In-Situ Thermal Processing of Oil Shale/Sands			
4.1	Development of CFD-based simulation tool for in-situ thermal processing of oil shale/ sands			
	Implementation of correct geometry representation in Star-CCM+	Jun-10	Mar-11	Reported in Q2 2011 report
	Obtaining a time-temperature history for all oil shale elements	Nov-10		Delayed due to time constraints of computational intensive simualtions
4.2	Basin-wide characterization of oil shale resource in Utah & examination of in-situ production models			
	Select dataset for use in validation/ uncertainty quantification of in-situ production modeling	Mar-10		Unlikely to complete due to lack of industrial support for sharing data
	Develop models with preliminary geomechanics & reactions	Jun-10	Jun-10	Reported in Q2 2010 report
	Revise/revisit the P-4 core description, adding XRF and isotopic work	Dec-10	Oct-10	Writeup included in topical report
	Describe one complete core, including XRF and isotopic work	Dec-10	Oct-10	Writeup included in topical report
	Complete a regional cross section and synthesis of the four described cores (two cores have been completed to date)	Mar-11	Apr-11	

ID	Title/Description	Planned Completion Date	Actual Completion Date	Milestone Status
4.3	Multiscale thermal processing (pyrolysis) of oil shale			

	Complete pyrolysis experiments at two different scales	Feb-10	Mar-10	Reported in Q1 2010 report
	Complete mass balances for oil/gas/coke at different scales	Apr-10	Apr-10	Reported in this quarterly report
	Develop preliminary kinetic model for oil shale pyrolysis	Jun-10	Sep-10	Reported in Q2 2010 report & in paper manuscript
	Develop compositional representation of shale oils	Sep-10	Nov-10	Reported in this quarterly report
	Design experiments for performing pyrolysis under stress	Nov-10	Dec-10	Reported in this quarterly report
4.4	Effect of oil shale processing on water compositions			
	Complete preliminary analysis of process water, including some tables of aqueous phase organic species concentrations	Nov-10	Nov-10	Reported in Q1 2011 report
	Determine compositional impact on reservoir scale of soluble pyrolysis products	Dec-10	Mar-11	Reported in this quarterly report
4.5	Pore scale analysis of oil shale/sands pyrolysis			
	Perform XMT/XNT analysis of samples of pyrolysis products at different temperatures	Jun-10	Jun-10	
	Model pore network structure at different heating rates to determine porosity changes	Sep-10	Oct-10	Delayed because samples not received from Subtask 4.3
	Use multiphase LB model to analyze fluid penetration into porous samples & to provide transport information such as connectivity, conductivity, & permeability	Dec-10	Dec-10	
4.6	Kerogen/asphaltene/mineral matrix: structure & interactions			
	Develop 3D models of kerogen & asphaltenes based on existing 2D models	Mar-10	Mar-10	Reported in Q1 2010 report

ID	Title/Description	Planned Completion Date	Actual Completion Date	Milestone Status

	Calculate interaction energies between organic components & mineral matrix using 3D models	Sep-10	Sep-10	Reported in Q3 2010 report
	Correlate spectroscopic data of isolated & absorbed 3D models, establish sensitivity to model structural features	Nov-10	Nov-10	
5.0	Environmental, Legal, Economic, & Policy Framework			
5.1	Land & resource management issues relevant to deploying in-situ thermal technologies			
	Detailed outline & abstract adressing land & resource management issues	Sep-10	Sep-10	
5.2	Policy analysis of water availability & produced water issues associated with in-situ thermal technologies			
	Detailed outline & abstract addressing produced water issues	Aug-10	Sep-10	
6.0	Economic & Policy Assessment of Domestic Unconventional Fuels Industry			
6.1	Engineering process models for economic impact analysis			
	Identify & describe selected scenarios & methodology applied to obtain associated upstream supply costs	Feb-10	Feb-10	
	Deliver upstream supply costs & listing of materials, equipment & services needed for facility construction & on-going operations & maintenance for each scenario	May-10	Jun-10	Spreadsheet of results included as attachment with Q2 2010 report
	Upload all models used & data collected to repository	Oct-10		Change from vertical to horizontal drilling has delayed completion
6.2	Policy analysis of the Canadian oil sands experience			
	Preliminary report addressing differences between U.S. & Canada in terms of taxes and royalties levied on production & in downstream/marketing challenges (to be incorporated into final report)	Jun-10	Jun-10	Included as appendix to Q2 2010 report

ID	**Title/Description**	**Planned Completion Date**	**Actual Completion Date**	**Milestone Status**

6.3	Market assessment report			
	Identify & describe criteria used to select scenarios for further study	Dec-09	Dec-09	Included as appendix to Q4 2009 report
	Identify & describe methodology applied to assess impact of downstream market conditions on potential revenue of upstream scenarios	Feb-10	Feb-10	Reported in Q1 2010 report
	Describe methodology & preliminary results of supply cost analysis for one scenario, including effect of system shocks or input variability	Apr-10	Dec-10	Will be released with rest of draft Market Assessment
	Deliver assessment of impacts to revenue corresponding to each scenario	May-10	Jun-10	Included as appendix to Q2 2010 report
	Preliminary report summarizing first three sections of Market Assessment (role of unconventional fuels in current energy climate; role of policy & government, role of externalities & public perception	Sept-10	Dec-10	Reported in this quarterly report

NOTEWORTHY ACCOMPLISHMENTS

The work completed for Subtask 4.2 provides a geologic framework for the next phase of engineering, chemical and geomechanical investigation of the Skyline 16 core in which stratigraphic variations in oil shale qualities (oil shale richness and mineralogy) will be compared in terms of pyrolysis products, chemical properties, geomechanics in order to determine if these geologic variations are significant considerations in potential oil shale development. Additionally, this work has resulted in the recognition of paleoclimatic control on oil shale accumulation and distribution, which has previously been underappreciated in this ancient lake system.

PROBLEMS OR DELAYS

The topical report for Subtask 3.1 detailing results of lifecycle GHG emissions from a refinery or upgrader using conventional & oxy-fuel flameless technologies will continue to be delayed while the Task 6.1 scenarios are finalized.

For Subtask 3.2, the V/UQ analysis continues to be delayed by the time constraints of the PI. This problem will be alleviated once the Market Assessment has been completed.

The Subtask 4.1 milestone to obtain a time-temperature history of all oil shale elements has been delayed due to researchers concentrating on finding the effects of boundary conditions on the thermal history of the fluid inside of the domain. As a result, they have postponed their computationally intensive simulations involving both fluid and solid phases and are testing boundary condition effects in an idealized computational system. Reporting on the time-temperature history of all oil shale elements will be found in the upcoming topical report.

Subtask 4.6 researchers have been hampered by the availability of experimental data, especially with respect to the publication of their paper entitled “Three-dimensional structure of the Siskin Green River oil shale kerogen model: A computational study.” As reported here, team members are just now starting to get samples on which experimental data can be obtained.

The Subtask 6.1 deliverable of a topical report describing process models for unconventional fuel production and the Subtask 6.3 deliverable of a draft Market Assessment report are directly linked. Due to continued refinement of the Subtask 6.1 process models, the Market Assessment draft wasn’t released prior to the end of this quarter.

RECENT AND UPCOMING PRESENTATIONS/PUBLICATIONS

J. H. Bauman and M. D. Deo, “Simulation of a rubblized oil shale surface pyrolysis process,” 30th Oil Shale Symposium, Colorado School of Mines, Golden, CO, October 18-20, 2010.

J. H. Bauman, P. Mandalaparty, P. Tiwari, and M. D. Deo, “A low CO2 hybrid in situ oil shale liquid production process,” 30th Oil Shale Symposium, Colorado School of Mines, Golden, CO, October 18-20, 2010.

L. Birgenheier and M. Vanden Berg, “Detailed geologic characterization of the Upper Green River Formation, Uinta Basin, UT,” 30th Oil Shale Symposium, Colorado School of Mines, Golden, CO, October 18-20, 2010.

P. Tiwari and M. D. Deo, “The effect of pressure on oil shale thermal treatment,” 30th Oil Shale Symposium, Colorado School of Mines, Golden, CO, October 18-20, 2010.

J. H. Bauman and M. D. Deo, “Relationship between kinetic and flow parameter representations in complex in situ reactive processes,” AICHE Annual Meeting, Salt Lake City, UT, November 7-12, 2010.

K. E. Kelly, T. Ring, J. Wilkey, B. Castro, A.F. Sarofim, and D.W. Pershing, “Opportunities for oxyfiring to reduce upstream life-cycle greenhouse gas emissions from transportation fuels,” AIChE Annual Meeting, Salt Lake City, UT, November 7-12, 2010.

B. Isaac, M. Hradisky, P. Smith, “Development of CFD-based simulation tools for in-situ thermal processing of oil shale/sands,” AICHE Annual Meeting, Salt Lake City, UT, November 7-12, 2010.

P. Tiwari and M. Deo, “Thermal gravimetric – mass spectrometry analysis of oil shale,” AICHE Annual Meeting, Salt Lake City, UT, November 7-12, 2010.

C. L. Lin, J. D. Miller, and C. H. Hsieh. “Flow simulation with the Lattice Boltzmann method in 3D porous structures of pyrolyzed oil shale cores using multiscale X-Ray CT imaging,” AICHE Annual Meeting, Salt Lake City, UT, November 7-12, 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,” *Flow Measurement and Instrumentation*, 21 (2010) 255-261.

J. H. Bauman and M. D. Deo. Parameter space reduction and sensitivity analysis in complex thermal subsurface production processes, *Energy Fuels*, 25 (2011) 251–259.

K. P. Tiwari and M. Deo, “Detailed kinetic analysis of oil shale pyrolysis TGA data.” AICHE Journal, 57 (2011).

K. P. Tiwari and M. Deo, “Compositional and kinetic analysis of oil shale pyrolysis using TGA-MS.” Submitted to *Fuel*, April 2011.

I. S. O. Pimienta, Badu, A. M. Orendt, J. C. Facelli, and R. J. Pugmire, ”Ab initio calculation and molecular dynamics simulation of asphaltenes.” Submission to *Energy & Fuels*.

I. S. O. Pimienta, A. M. Orendt, R. J. Pugmire, 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.” Publication of manuscript has been delayed pending acquisition of experimental data.

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Campbell, J. H., Koskians, G. J., Coburn, T. T., Stout, N. D. (1978) Oil shale retorting: The effects of particle size and heating rate on oil evolution and intraparticle oil degradatio, *In - Situ*, *2*, 1-47.

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

Siskin, M., Kelemen, S. R., Eppig, C. P., Brown, L. D., & Afeworki, M. (2006). Asphaltene molecular structure and chemical influences on the morphology of coke produced in delayed coking, *Energy & Fuels, 20*, 1227-1234.

APPENDIX A. Conference Agenda and Field Trip Itinerary

UNIVERSITY OF UTAH
UNCONVENTIONAL FUELS CONFERENCE
2011

AGENDA

8:30 a.m. Welcome/opening remarks – Philip J. Smith, Director, Institute for Clean and Secure Energy, Professor, Department of Chemical Engineering, University of Utah

Session 1: Utah Regulatory and Economic Landscape for Unconventional Fuels Development

8:40 a.m. "State Permitting Process for Unconventional Fuels" – John Baza, Director, Utah Division of Oil, Gas, and Mining

9:10 a.m. "Air Quality Constraints in the Uinta Basin" - Bryce Bird, Branch Manager, Utah Division of Air Quality

9:40 a.m. – "Balancing Economic Development in the Energy Sector and Quality of Life" – Spencer Eccles, Executive Director, Utah Governor's Office of Economic Development

10:10 a.m. Break; display of newly drilled Skyline 16 core

Session 2: Industrial Perspectives on Unconventional Fuel Development

10:40 a.m. "Red Leaf and the Regulatory/Commercialization Process" – Laura Nelson, Vice President, Energy and Environmental Development, Red Leaf Resources

11:10 a.m. "AMSO RD&D Lease" – Alan Burnham, Chief Technology Officer, American Shale Oil

11:40 a.m. "Uintah Partners, LLC. Wax Crude Upgrading Facility" – Vince Memmott, Uintah Partners

12:00 p.m. Lunch; display of newly drilled Skyline 16 core

Session 2 (continued):

1:00 p.m. "Introduction to Enefit" - Harri Mikk, Chairman of the Board, Enefit American Oil

1:30 p.m. "Project Transition from Technology Development to Operational Deployment" – D. Glen Snarr, President and Chief Financial Officer, Earth Energy Resources

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2:00 p.m. Break; display of newly drilled Skyline 16 core

Session 3: Planning for Unconventional Fuels Development

2:20 p.m. “Federal Oil Shale Development: Status of Bureau of Land Management Oil Shale Activities” – Mitchell Leverette, Chief, Division of Solid Minerals, Washington D.C. Office, Bureau of Land Management

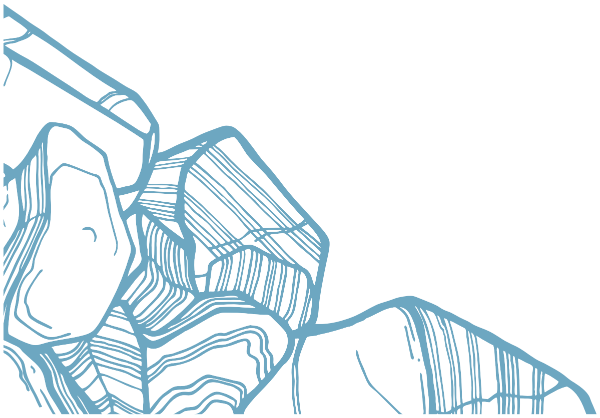
2:50 p.m. “Wild Lands and Wilderness - Implications for Utah’s Unconventional Fuels Industry“ – John Ruple, Research Associate, Institute for Clean and Secure Energy, University of Utah

3:20 p.m. “Unconventional Fuels Development and the Environment” – Robert Bayer, President, JBR Environmental Consultants

3:50 p.m. “Energy Development on Tribal Lands” – Cameron Cuch, Vice President, Government Affairs and Corporate Development, Ute Energy, LLC

Session 4: Plenary

4:15 p.m. “Climate Change Regulation via the Back Door” – Arnold W. Reitze, Jr., Professor, S. J. Quinney College of Law, University of Utah



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Itinerary for 2011 Uinta Basin Field Trip

Wednesday, 18 May

7:30 a.m.	Meet at Department of Natural Resources, 1594 W. North Temple
8:00 a.m.	Leave Salt Lake City
12:00 p.m.	Eat lunch at Bingham Energy Research Center (BERC)
12:30 p.m.	Board bus at BERC
1:00 p.m.	Tour of oil rig & fracing operation
5:00 p.m.	Tour of BERC
6:30 p.m.	Dinner at BERC
8:00 p.m.	Spend the night at Springhill Suites/Holiday Inn Express

Thursday, 19 May

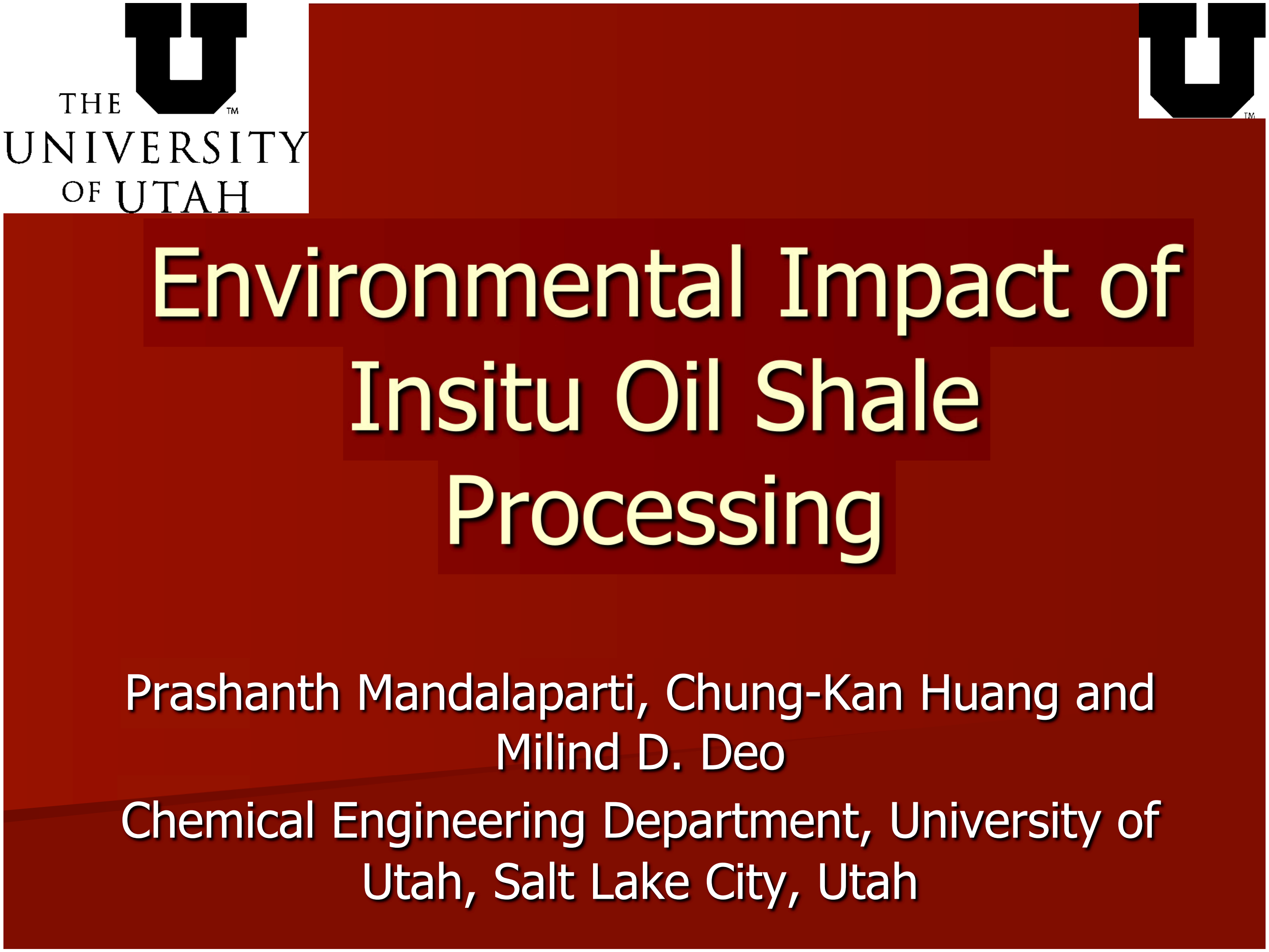
7:30 a.m.	Continental breakfast at the hotel
8:00 a.m.	Leave Vernal
8:15 a.m.	Tour of Enshale
9:15 a.m.	Tour of Asphalt Ridge oil sands pit
11:00 a.m.	Tour of Enefit's White River Mine site
12:00 p.m.	Lunch at White River Mine
1:30 p.m.	Geology stop at Evacuation Creek
2:45 p.m.	Geology stop at Mahogany Outcrop
4:30 p.m.	Arrive in Vernal
8:00 p.m.	Arrive in Salt Lake City

APPENDIX B. Project Review Meeting, 10-11 March 2011, University of Utah campus

Thursday, March 10
8:30 a.m. - Subtask 5.1: Land and resource management issues relevant to deploying in situ thermal technologies
9:15 a.m - Subtask 5.2: Policy analysis of water availability and produced water issues associated with in situ thermal technologies
10:00 a.m. - Subtask 6.2: Policy analysis of Canadian oil sands experience
10:45 a.m. - Break
11:00 a.m. - Subtask 4.6: Kerogen/Asphaltene/Mineral Matrix: Structure and Interactions
11:45 a.m. - Subtask 4.5: Pore scale analysis of oil shale/sands pyrolysis
12:30 p.m. - Lunch
1:15 p.m. - Subtask 4.3: Multiscale thermal processing (pyrolysis) of oil shale
2:00 p.m. - Subtask 4.4: Effect of oil shale processing on water composition
2:45 p.m. - Break
3:00 p.m. - Subtask 3.1: Macroscale CO2 analysis
3:45 p.m. - Subtask 6.1: Engineering process models for economic impact analysis
4:30 p.m. - Subtask 6.3: Market Assessment Report
5:15 p.m. - Adjourn for the day

Friday, March 11
8:30 a.m. - Subtask 3.2 - Flameless oxy-gas process heaters for efficient CO2 capture
9:15 a.m. - Subtask 4.1: Development of CFD-based simulations tool for in situ thermal processing of oil shale/sands
10:00 a.m. - Break
10:15 a.m. - Subtask 4.2(A): Basin-wide characterization of oil shale resource in Utah
11:00 a.m. - Subtask 4.2(B): Examination of in-situ production models
11:45 a.m. - Adjourn

APPENDIX C. Environmental Impact of In Situ Oil Shale Processing



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Environmental Impact of Insitu Oil Shale Processing

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