Oil & Natural Gas Technology

DOE Award No.: DE-FE0001243

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

Quarterly Progress Report (July - September)

Submitted by:
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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
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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 cosponsored the 2011 Energy Forum, which was held in the Gould Auditorium at the Marriott Library on the University of Utah campus. The panelists for this year's event were former Senator Bob Bennett, former Wyoming Governor Dave Freudenthal, and James Holtkamp, Esq., Climate Change Practice Team Leader at Holland & Hart. Plans were also made to convene a reconstituted External Advisory Board on November 1-2, 2011.

Researchers in Task 3.0 continued to gather information on Uinta Basin oil and gas production from well completion reports and from production data available from the Utah Division of Oil, Gas, and Mining website. The well completion reports show that drilling costs are a strong function of well depth but relatively independent of well type (oil or gas). Additional information was collected on produced water disposal in the basin. Very little treatment is performed on produced water. It is either reinjected to stimulate further production or sent to evaporations ponds. Researchers also developed a preliminary module for the oil and gas production processes.

Subtask 3.2 researchers have modified the ARCHES large eddy simulation tool to better capture the inputs and output of interest for the pilot-scale, oxy-gas fired furnace that is the focus of a validation/uncertainty quantification study. These changes include a swirl model, a thermal NO_x model, and improved models for the burner geometry and for heat exchange with the walls. The variable is most industrial interest is NO_x emissions due to NO_x regulations being promulgated by the U.S. Environmental Protection Agency.

Research and analyses on three different sections of the Skyline 16 core (GR-1, GR-2, and GR-3) are the focus of several projects under Task 4.0. Subtask 4.3 researchers have performed thermogravimetric analysis experiments on the core samples at both atmospheric pressure and at 40 bar on small cores and on powdered samples. Subtask 4.5 researchers have examined the core samples using 3D multiscale X-ray computed tomography analysis. Research performed during this quarter involved Skyline 16 oil shale cores. Their goal is to better understand pore scale transport processes in the pyrolysis of oil sands and oil shale. Subtask 4.7 researchers pressure tested the apparatus they will be using to determine geomechanical properties of the Skyline 16 core samples. Finally, Subtask 4.9 researchers are demineralizing kerogen samples for subsequent C-13 NMR analsysis. The original demineralization process had to be modified when it was discovered that significant quantities of mineral matter still remained in the "demineralized" samples.

In other Task 4.0 projects, Subtask 4.1 researchers continued to improve their computational representation of the rubblized shale geometry and have coupled their newly developed operator splitting numerical algorithm with a computational domain representative of that used by Red Leaf Resources in their ECOSHALE capsule. Subtask 4.2 team members focused on improving the geomechanical modeling of in situ oil shale production processes by exploring the capabilities of the Material Point Method as implemented in the Uintah Computational Framework and of the geomechanical model options in the commercially available STARS software. Subtask 4.6 researchers developed optimized 3D structures for the mid-continent asphaltene. Lastly, the Subtask 4.8 team completed drafting the sedimentary log of the Skyline 16 core.

Subtask 5.1 researchers continued drafting portions of the topical report examining issues associated with wilderness quality land management, its implications for unconventional fuel

developers, and potential paths forward. Subtask 5.2 team members completed research on conjunctive surface water and groundwater management in Utah and are drafting the topical report.

In Task 6.0, the project team finalized details of the four unconventional fuel development scenarios in Utah's Uinta Basin. Extensive revisions were made to the draft report based on feedback from reviewers. Because of intense media scrutiny, the project team is carefully reviewing the assumptions, methodologies, and sources for each scenario prior to publications. Subtask 6.2 researchers are preparing a topical report contrasting Canadian oil sands development and potential domestic oil sands development.

The Strategic Alliance Reserve set aside for Task 7.0 to fund collaborative projects with industry has been parsed out to three projects that were developed in consultation with the industrial partner, American Shale Oil (AMSO). The three projects are a geomechanical model of the non-linear stress-strain relationships for oil shale with specific reference to AMSO properties, kinetic compositional models incorporated into thermal reservoir simulators to more realistically represent all the complex processes during oil shale pyrolysis and subsequent production of multiple phases, and rubblized bed high performance computing simulations that can resolve the scale of the individual rubblized pieces of shale. A work statement with timelines, milestones, deliverables, and budgets as been submitted to the Department of Energy.

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. However, new subtasks under Task 7.0, the Strategic Alliance Reserve, were added in this quarter, so the PMP will be amended in the next quarter.

Task 2.0 -Technology Transfer and Outreach

Task 2.0 focuses on outreach and education efforts and the implementation of External Advisory Board (EAB) recommendations. During this quarter, ICSE and the Wallace Stegner Center for Natural Resources and the Environment co-sponsored the 2011 Energy Forum. It was held on Wednesday, September 14, 2011 in the Gould Auditorium at the Marriott Library on the campus of the University of Utah. The panelists for this year's event were former Senator Bob Bennett, former Wyoming Governor Dave Freudenthal, and James Holtkamp, Esq., Climate Change Practice Team Leader at Holland & Hart. Approximately 200 people attended this year's Energy Forum. The event was also streamed live and recorded for posting on the ICSE and Stegner Center websites and inclusion in the Marriott Library's Special Collections. A copy of the promotional flyer for the event is attached as Appendix A.

EAB efforts this quarter focused on sending updated project information to EAB members as well as corresponding with EAB members regarding changes to the composition of the Board. The 2011 EAB meeting, which will convene the reconstituted EAB, will be held on November 1-2, 2011. A preliminary draft of the EAB meeting agenda is attached as Appendix B. A copy of the 2011 Advisory Board Update is attached as Appendix C. Current EAB members are Ian Andrews of PacifiCorp, Spencer Eccles of the Utah Governor's Office of Economic Development, James Holtkamp of Holland & Hart, Sho Kobayashi of Praxair, Robert Lestz of GasFrac, John Marion of Alstom, Dianne Nielson, formerly the Governor's Energy Advisory for the State of Utah, Laura Nelson of Red Leaf Resources, David Pershing, Distinguished Professor and Senior Vice President for Academic Affairs at the University of Utah and Director of the EAB, Mark Raymond, Uintah County Commissioner, and Adel Sarofim, Presidential Professor at the University of Utah. Madhava Syamlal of NETL has been identified and approached as a possible replacement for Joseph Strakey of NETL who has retired from NETL and resigned from the EAB.

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

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

Due to delays in completing Subtask 6.1, the final deliverable for this subtask will not be completed until October 2011.

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

During this quarter, Subtask 3.1 researchers continued to refine their understanding of oil and gas operations in the Uinta Basin, to collect relevant greenhouse gas (GHG) emission factors, and to understand the $CLEAR_{uff}$ model and the Anylogic software. Some time was devoted this quarter to assisting Subtask 3.4 with collection of data from well completion reports including costs, well depth, and fuel usage. Some of this data will be important to the GHG emission modules.

Several potentially useful GHG data sources were identified, and the Subtask 3.1 team is in the process of reviewing and organizing the data for integration into the $CLEAR_{uff}$ modules. As an example, researchers extracted the annual Utah-specific electricity resource mix from the US Energy Information Administration (EIA) datasets (Table 1) and simplified it for use in the $CLEAR_{uff}$ model. The simplifications included grouping petroleum and other gases, which comprises less than 0.2% of the resource mix, with natural gas. Renewables include geothermal, biomass, and wind. Biomass comprises less than 0.1% of the resource mix. The EIA data shown in Table 1 agree with the Environmental Protection Agency's e-grid data, although e-grid is only available for 2005 and 2007. The team also gathered information on line losses in the region, and this information as well as average GHG emission factors for Utah's resource mix are available on the project wiki under air quality.

Table 1. Simplified Utah annual average electricity resource mix, by percent.

	2001	2002	2003	2004	2005	2006	2007	2008	2009	2010
Coal	93.9%	94.2%	94.6%	95.8%	94.2%	89.3%	81.9%	81.6%	81.6%	80.7%
Natural Gas	4.2%	3.1%	3.7%	2.5%	3.2%	8.4%	16.5%	16.0%	15.0%	15.2%
Hydroelectric	1.4%	1.3%	1.1%	1.2%	2.1%	1.8%	1.2%	1.4%	1.9%	1.9%
Renewables	0.5%	0.6%	0.5%	0.5%	0.5%	0.5%	0.4%	1.0%	1.5%	2.2%

Other resources currently being reviewed for relevant data include a drilling rig emission inventory published by the Texas Commission on Environmental Quality and a study by the Western Regional Air Partnership on transportation-related air emissions associated with oil and gas production in the Piceance Basin. In addition, the Utah Department of Environmental Quality is working on an updated oil and gas emission inventory (results expected in the fall of 2012) and the US Bureau of Land Management will be publishing another potentially relevant inventory in the next few months.

The team also devoted some time to modifying the electricity mix options in the $CLEAR_{uff}$ model to support a Utah grid mix in addition to the Colorado grid and a Western regional grid.

However, the project team has decided to develop a simplified $CLEAR_{uff}$ model for use in oil and gas, and the electricity module will need to be rebuilt from scratch as part of that effort.

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

Subtask 3.2 researchers identified the output variables of interest for the validation/uncertainty quantification (V/UQ) analysis of the oxy-gas experiments conducted by the by the International Flame Research Foundation or IFRF (Coraggio and Laiola, 2009). These output variables include NO_x concentration, CO_2 concentration, O_2 concentration, and local gas temperature. NOx concentration is of most interest to companies who are considering alternative combustion technologies because the U.S. Environmental Protection Agency is promulgating new NO_x regulations. In contrast, the interest in oxy-firing for CO_2 capture has waned somewhat due to the lack of any clear direction at the federal level on CO_2 regulation.

The scenario, model, and numerical parameters that are most likely to influence NO_x concentrations include the burner geometry, the degree of swirl in the burner, and the O_2 concentration in the inlet stream(s). Subtask 3.2 researchers located additional details and photos of the IFRF TEA-C burner (see Figure 1) that clarified some questions regarding the burner geometry that weren't clear from design drawings (Corraggio et al., 2011), including the collocation of the primary stream and the fuel jets and presence of flanges that significantly reduce the exit surface area of the secondary and tertiary streams. However, despite this new information regarding the burner geometry, the inlet velocity vectors (degree of swirl) are still unknown. Hence, Subtask 3.2 researchers are taking a two-pronged approach. First, simulations are being performed in the large eddy simulation tool ARCHES with swirl number as one of the parameters in the test matrix. Second, the burner itself is being modeling in the commercial software Star-CCM+ (see Subtask 4.1 summary). If this effort is successful, the velocity profiles at the burner exit obtained from the Star-CCM+ simulation will be used as the velocity inlet condition for the ARCHES simulations.

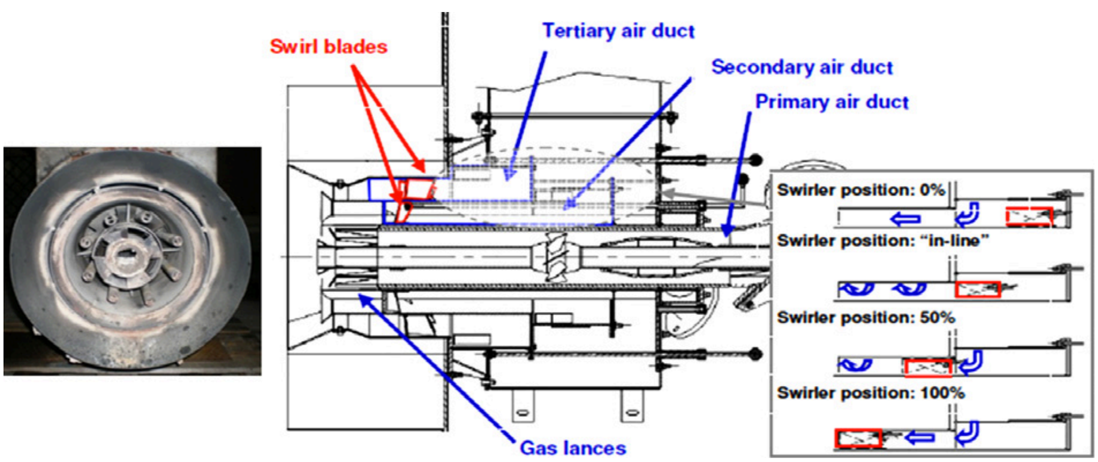


Figure 1: Photo of the TEA-C burner with a cross-section of the TEA-C burner and the swirler position scheme; from Corraggio et al., 2011.

Additional software development was required to perform ARCHES simulations with swirl and to more accurately predict NO_x chemistry. In this quarter, Subtask 3.2 researchers added a swirl model and a thermal NO_x model to ARCHES. Some bugs with respect to the furnace wall boundary condition were also fixed. All new models underwent a thorough verification process.

ARCHES simulations are being performed for a range of swirl numbers. The computational domain for all simulations is 4m x 2.1m x 2.1m with 0.05 m thick walls. For these simulations, the burner geometry in ARCHES has been modified to better approximate the actual TEA-C geometry. These modifications include annular blockages in the primary and secondary streams and a reduction in the annular width of the tertiary stream. The simulations require 1,024 cores and are being run on a massively parallel machine at the University of Utah. Figure 2 shows the temperature field in a slice through the middle of the domain after approximately 0.2 s of simulation time for a simulation where the swirl number was set to two. The effect of swirl is to introduce more rapid mixing near the burner. Work is ongoing to determine the range of swirl numbers that brackets the region of consistency between the experimental and simulation data.

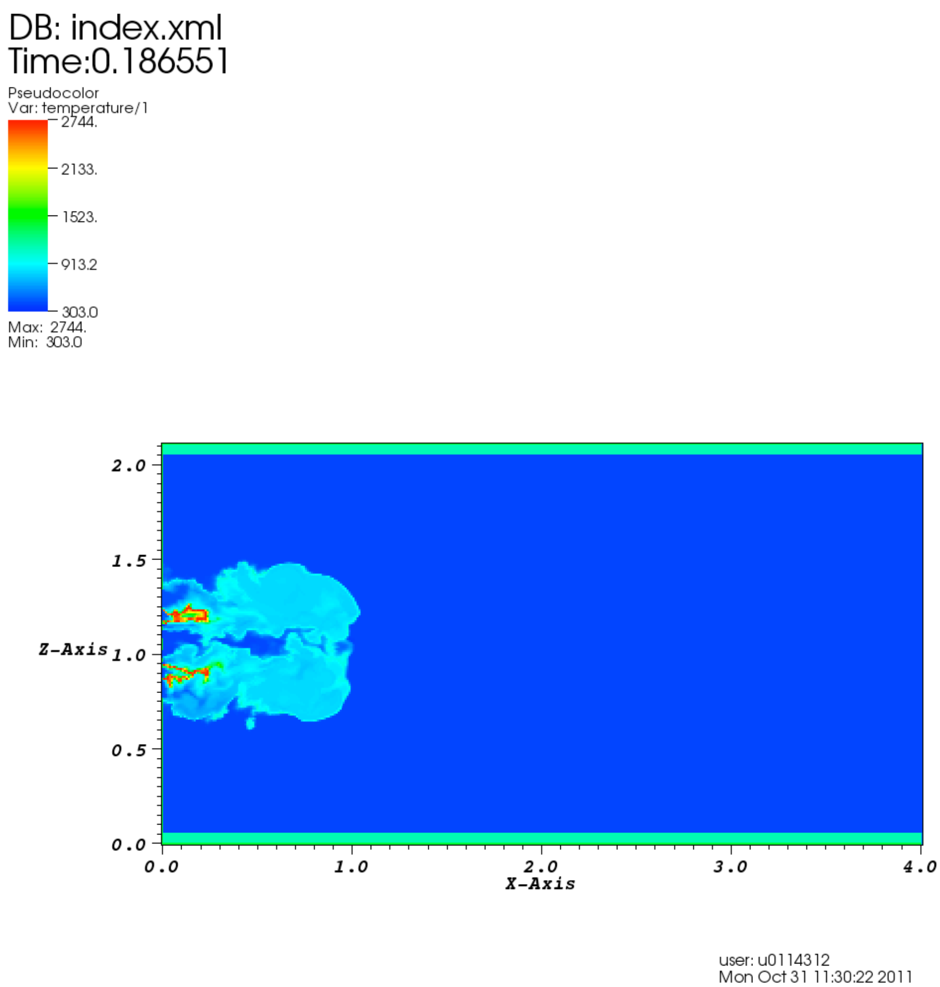


Figure 2: Slice through the middle of the temperature field from a simulation of the IFRF furnace fired with a TEA-C burner. Swirl number is two.

Subtask 3.3 - Development of Oil and Gas Production Modules for $CLEAR_{uff}$ (PI: Terry Ring)

During the quarter, the Subtask 3.3 project team has been gathering information for the produced water aspects of oil and gas recovery in the Uinta Basin. Produced water comes from two sources: (1) fracking of deposits to make them more productive and (2) normal production.

Produced water from fracking can be a significant portion, ~20-30%, of the million gallons typically used in a fracking operation, but it is a one time production of water. In the Uinta Basin, fracking produced water is typically sent to evaporation ponds for disposal. Produced water from normal production is by far the largest source of produced water as it comes continuously from the production of the well. Generally, this type of produced water is reinjected in the same oil or gas reservoir to help stimulate further production. With each production well there are injection wells that are associated with it. However, there is more produced water than needed by reinjection wells, resulting in an excess of produced water. Produced water from normal production typically has high concentrations of dissolved salts and traces of oil and gas. In the Uinta Basin, excess produced water is typically sent to evaporation ponds for disposal. Data on water production from oil and gas wells is available from the Utah Division of Oil, Gas, and Mining (DOGM) database.

The team has identified the surface processing methods employed at the gathering stations for both oil and gas. For oil production, the oil and produced water are typically pumped into a tank at the well head. Communications between this automated tank and the base station send tankers when needed to empty the tank of either water or oil or both. The tanker transports the produced water to a gathering plant where it is treated to remove the oil and gas. The water is then passed to a froth flotation cell followed by a sand bed filter before it is sent to the evaporation pond. For gas production, a three phase flash unit at the well head allows clean gas to be piped to the gathering plant. The produced water is typically tanked and periodically transported to a central gathering plant for clean up.

Mass and energy balance models of the various produced water separation units are being developed in an attempt to understand the capital and operating costs as well as the various types of energy utilized on a per gallon basis for implementation into the $CLEAR_{uff}$ model.

<u>Subtask 3.4 - V/UQ Analysis of Basin Scale $CLEAR_{uff}$ Assessment Tool (PI: Jennifer Spinti)</u>

The Subtask 3.4 team developed a preliminary module for the oil and gas production process, a milestone that is listed for completion in October 2011. The module does not yet incorporate yet the data inputs that have been gathered from well completion reports. Additionally, the project team began to reframe the $CLEAR_{uff}$ model by building a library of modules so that a version control system can be applied to the model. Version control will allow several developers to collaborate simultaneously on the same model.

Well completions reports available from the DOGM database are being mined for information on drilling depth, time required, drilling costs, and inputs required (fuel, water, electricity). Because of the wide range in quality of these reports, only those companies with the most complete set of information are included in the analysis. Fortunately, that group includes some of the biggest drillers in the Uinta Basin. A summary of the data that has been collected and analyzed thus far is attached to this report as Appendix D.

Finally, production data from the DOGM website is being used to generate production models for oil, gas, and produced water as a function of field and of well depth. Figure 3 shows the production curves of oil, gas, and water for all oil wells and gas wells that were spud dry in Uintah County between the years 2003-2005 and whose status was “producing”; this dataset include 90 oil wells and 326 gas wells. On the y-axis of the plots are production quantities; on the x-axis are the counts of months from the spud dry date. Hence, each production curve is plotted from month zero when in reality the wells were started at different times. Normalizing the data like this shows the general shape of the production curves for each type of well.

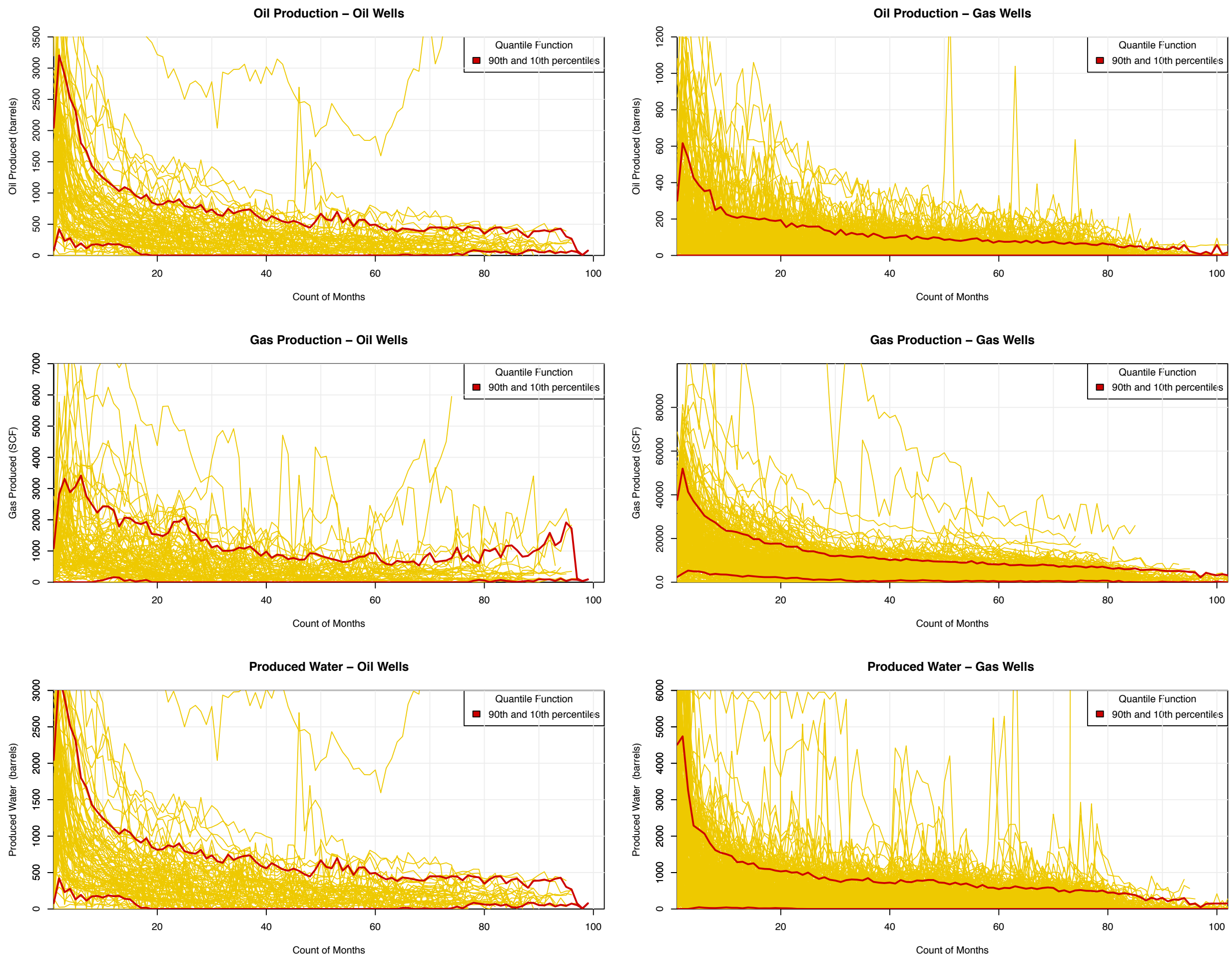


Figure 3: Oil, gas, and water production from producing oil and gas wells in Uintah County, Utah that were spud dry between 2003 and 2005.

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

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

The project team for Subtask 4.1 is using the Star-CCM+ commercial software package to develop a high-performance computing simulation tool that employs computational fluid dynamics (CFD) to study in-situ thermal processing of oil shale. During this quarter, team members have continued to improve their computational representation of the rubblized shale geometry and have coupled their newly developed operator splitting numerical algorithm with a computational domain representative of that used by Red Leaf Resources in their ECOSHALE capsule.

The geometry creation procedure used to approximate the rubblized pieces of oil shale inside the computational domain has been detailed in previous quarterly reports. Researchers use the DEM simulation capabilities of Star-CCM+ to create the representative rubblized pieces of the oil shale. The Star-CCM+ DEM simulation process is shown in Figure 4. The oil shale pieces are dropped into the computational section that represents the ECOSHALE capsule, including the heating pipes present in the actual geometry. The computational domain is 8 feet wide, 8 feet deep, and almost 18 feet tall (the actual height of the ECOSHALE capsule). We have selected the size of our computational domain such that it represents a periodical section of the ECOSHALE capsule.

With one exception, the project team continues to use the simplified geometric representation of the individual oil shale particles because of the meshing and the trapped internal volumes issues described in previous quarterly reports. That exception is the size of the particles. Previously, each individual particle of oil shale used to populate the computational domain was the same size. In this quarter, the complexity of the geometric representation has been increased by including two distinct oil shale particle sizes, as seen in Figure 5. Researchers continue to transition the geometry creation approach from Gambit to the ICEM CFD software package as Gambit is no longer commercially available. During transition, both software packages are used to create simulations that address the most urgent need of Red Leaf Resources – which is the time history of heating of each oil shale particle.

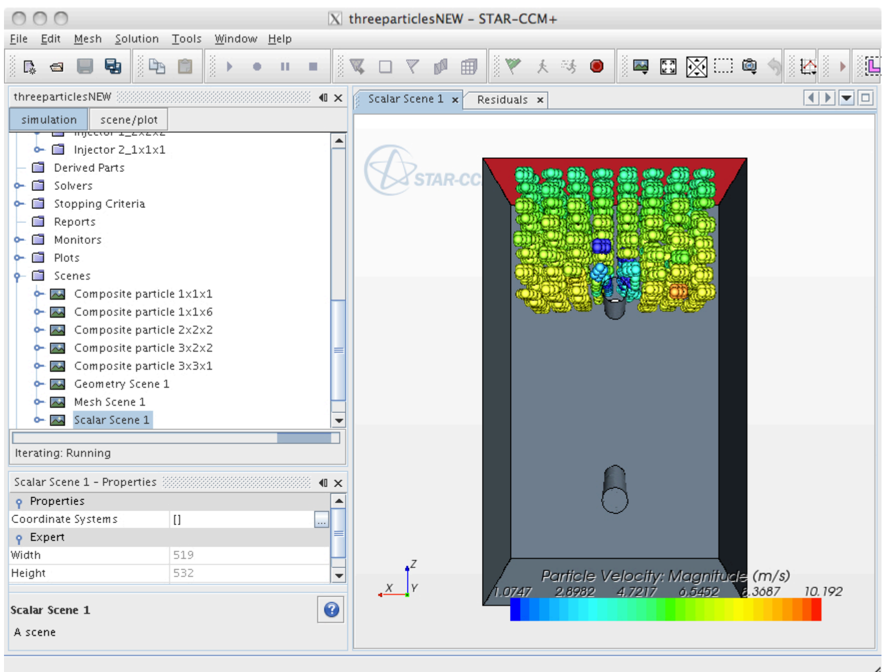


Figure 4: Star-CCM+ DEM simulation of a representative computational domain being filled with oil shale particles.

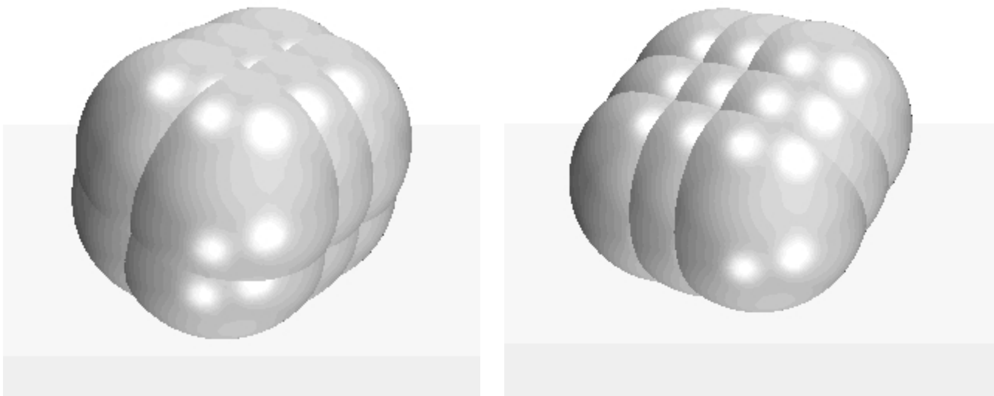
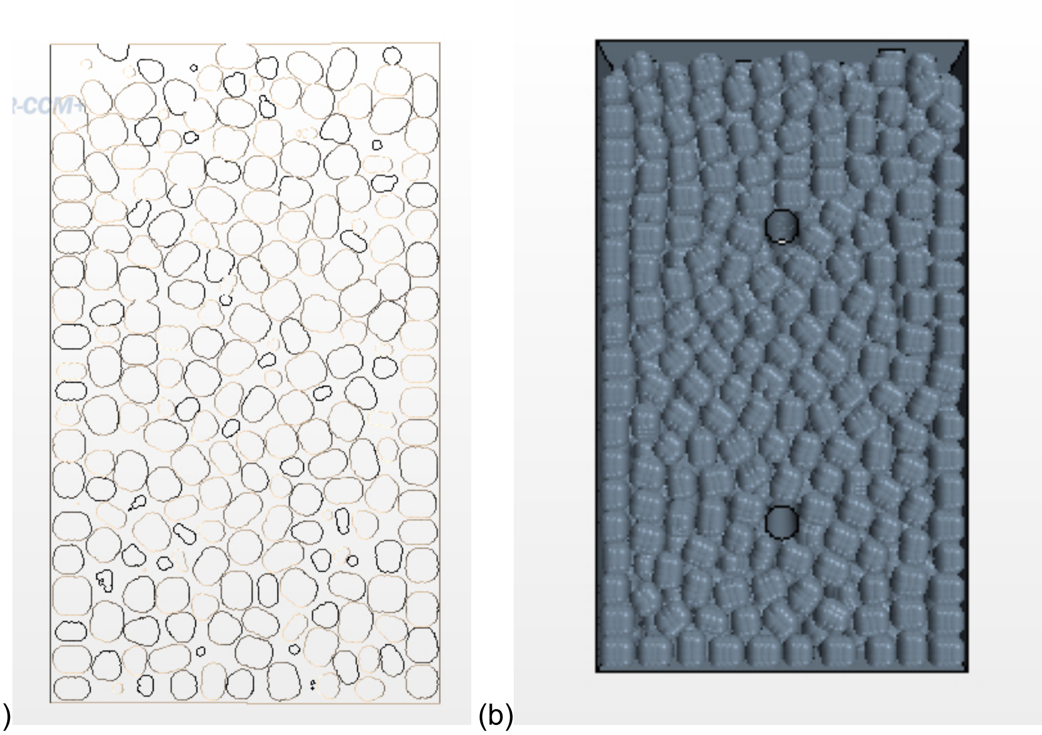


Figure 5: DEM representations of new oil shale particles of two different sizes.

Also this quarter, the project team has begun accounting for two adjacent solid particles that come into contact while creating the computational geometry. Instead of pure convective heat transfer, heat transfer with particles in contact uses a combined convection and conduction mode. This change is representative of the realistic oil shale packing inside the ECOSHALE capsule. Team members also continue to work on decreasing the size of the convective channels between pieces of oil shale such that the spacing is representative of channels in the actual rubblized oil shale bed. All these improvements to the geometric representation of othe computational domain can be seen in Figure 6.



(a) (b)

Figure 6: (a) Improved geometric representation of simulation domain that contains oil shale pieces of two different sizes with decreased sizes of convective heating channels between pieces of oil shale, as well as particles in contact, (b) three-dimensional graphical representation of the computational domain shown in (a)**.**

Finally, the project team has coupled their newly developed operator-splitting algorithm (detailed in the previous quarterly report) with the more complex geometrical representation of the computational domain. Previously, simulations required one day of computational time on 600 processors to produce one minute of simulation time. With the new operator splitting algorithm, one day of simulation time only requires about one day of computational time on 600 processors. The heat transfer inside the capsule at a simulation time of about 231,000 seconds (2.67 days) is shown in Figure 7. Simulation results predict that, in general, the capsule heats from top to bottom, following the path of the convective currents, and not radially, as one might have assumed.

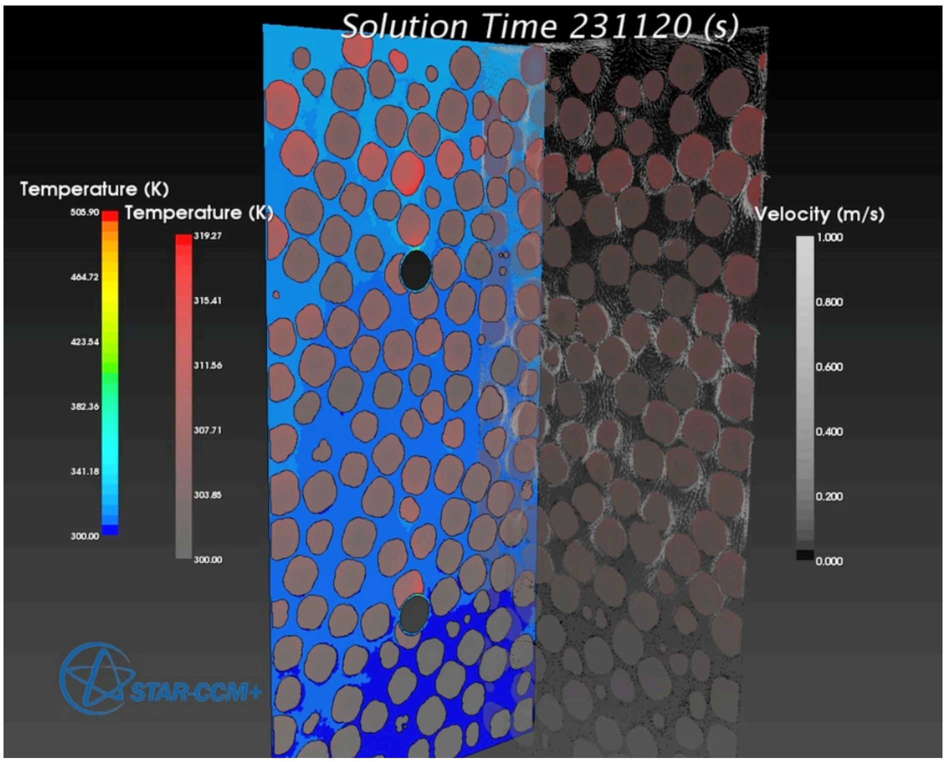


Figure 7: Heat transfer distribution inside a more complex geometric representation of the ECOSHALE capsule obtained using the operator splitting algorithm at a simulation time of about 2.67 days.

<u>Subtask 4.2 - Reservoir Simulation of Reactive Transport Processes (PI: Milind Deo)</u>

In this quarter, Subtask 4.2 researchers focused on improving the geomechanical modeling of in situ oil shale production processes. In 1980, the United States Office of Technology Assessment published *An Assessment of Oil Shale Technologies* (OTA, 1980). Only two in situ technologies were evaluated, true in situ (TIS) and modified in situ (MIS). TIS technology consisted of explosives being detonated underground to generate permeability. MIS technology consisted of the mining of a portion of the oil shale with underground mining techniques, followed by rubblization with explosives. A study of pilot scale processes in Wyoming (Goldstein, 1978) concluded that "calculations have shown that a minimum void volume of 10% is necessary to initiate and sustain in-situ combustion and retorting." If that void volume was not present, flow in the reservoir would not be possible. Current in situ retorting strategies by Shell, ExxonMobil, and AMSO do not include a rubblization step. Heating in these current processes is initially conductive, and permeable pathways are believed to be generated by solid kerogen conversion to fluids and by rock mechanical failure or fracturing. Understanding the geomechanics involved in such processes is important since oil shale resources are typically characterized by very low initial permeability.

In a paper by Tisot et al. (1970), the mechanical properties of oil shale subjected to heat and stress were evaluated. This paper concluded that "...kerogen ... is the predominant contributor to [rich oil shale] properties and to their response to heat and stress." Fragments of oil shale were placed in a stress environment and heated. It was found that "[i]n most instances the induced permeability in the column of fragments was reduced to zero." A final conclusion stated that "[t]his investigation shows that structural deformation in rich oil shales can be expected to occur ahead of the retorting zone." A similar study by Thomas et al. (1966) reported similar experiments with overburden pressure. The study concluded that thermal fracturing does not occur in an overburden environment, but some permeability is still generated by some other mechanism. Prats et al. (1977) performed experiments, including field tests, where nahcolite was solution mined from the oil shale prior to retorting, thus allowing heated oil shale to expand into void spaces and generate fractures. Solution mining of nahcolite created free surfaces where oil shale rock could fail by "stress release at open faces, thermally induced stresses, and thermally induced pressures." In *Oil Shale: A Solution to the Liquid Fuel Dilemma* (2011), AMSO states, "The shale ... will want to expand as it is heated, but since it is confined by the cool shale, it undergoes compressive failure and fills the high permeability conduit with rubble." AMSO also writes that "... the thermomechanical fragmentation process is expected to propagate out to retort diameters of 100 or more feet ..." In the same book, a chapter describing the Shell ICP states that "... it was hypothesized that bulk heating with thermal conduction would generate permeability and that the gases generated during retorting will drive liquid oil from the pores of the shale." Finally, ExxonMobil states, "... hydrocarbons will escape from heated oil shale even under in situ stress. … [Our] set of experiments clearly indicates that, even under conditions of overburden stress, the kerogen conversion and expulsion process creates porosity and permeability that was not present in the original oil shale" (Ogunsola et al., 2011). The current consensus by industry is that thermal stresses in oil shale will generate permeable pathways for fluids to flow.

Accurate geomechanical modeling will be important in situ oil shale process simulation. A simulation tool that has the capability of modeling thermal stresses, large material deformation, and mechanical failure due to stresses is the material point method (MPM). MPM was previously implemented in the Uintah Computational Framework (UCF), a framework developed at the University of Utah. Subtask 4.2 researchers have used the UCF implementation of MPM to simulate a 1 foot by 1 foot oil shale block where the bottom and side boundaries are confined. The top boundary is free to deform and move. The bottom boundary is suddenly subjected to a 1000°C temperature. Figure 8 shows the thermal stress profiles traveling through the block. Failure criteria can be added to MPM to approximate crack generation and propagation.

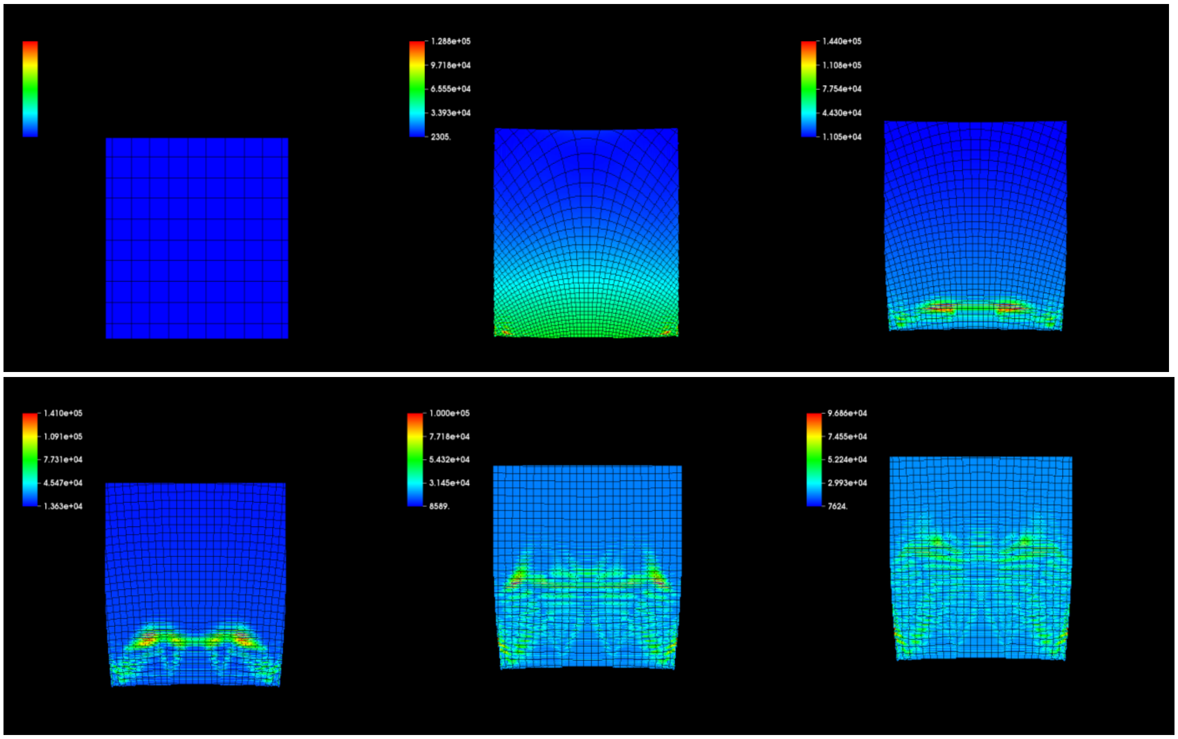


Figure 8: Thermal stress profiles in a two-dimensional UCF MPM simulation of a 1 foot x 1 foot oil shale block.

The role of geomechanics in in situ oil shale production was also studied using commercial software. Simulations were performed that utilized the STARS geomechanical module and a permeability/fluid porosity relationship shown in Equation 1.

$$k = k_0 \exp\left(k_{mul} \frac{\phi - \phi_0}{1 - \phi_0} \right) \qquad (1)$$

In these simulations, a 900 foot horizontal heater supplies heat to the oil shale resource with a horizontal producer at the bottom. The geometry used in the simulation is shown in Figure 9.

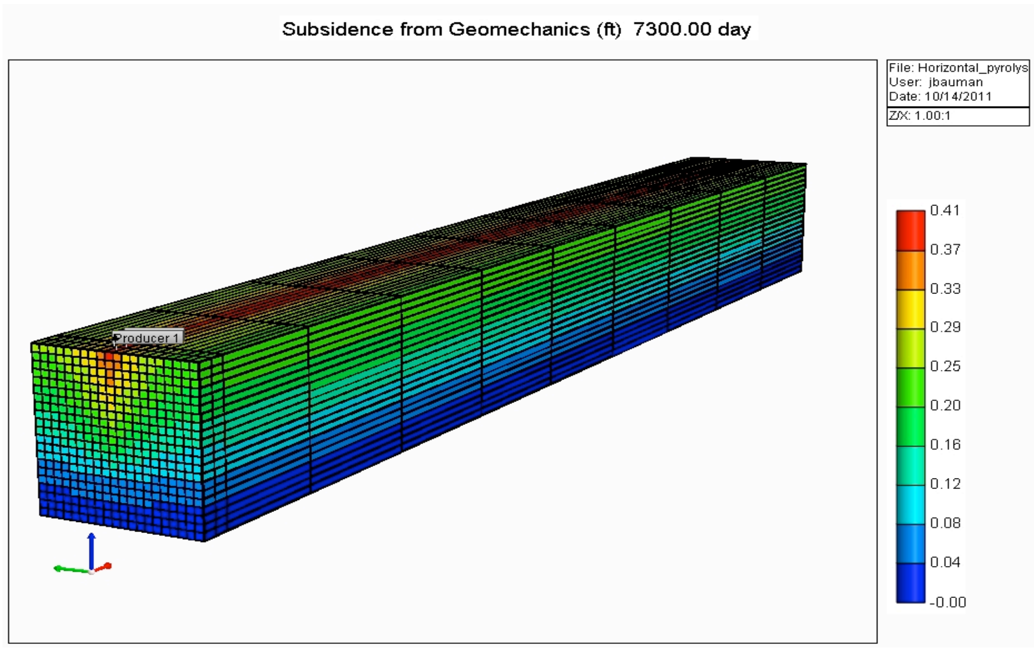


Figure 9: Geometry used in STARS simulation with geomechanics module. A horizontal heater supplies heat. A horizontal producer is located at the bottom.

Sensitivity studies were performed that considered the effect of the geomechanics module (with and without) and of a parameter in Equation 1 on oil production results. Results from these simulations are seen in Figure 10. It is clear that changes in the geomechanics module and in the permeability model in STARS make a significant difference in predicted results.

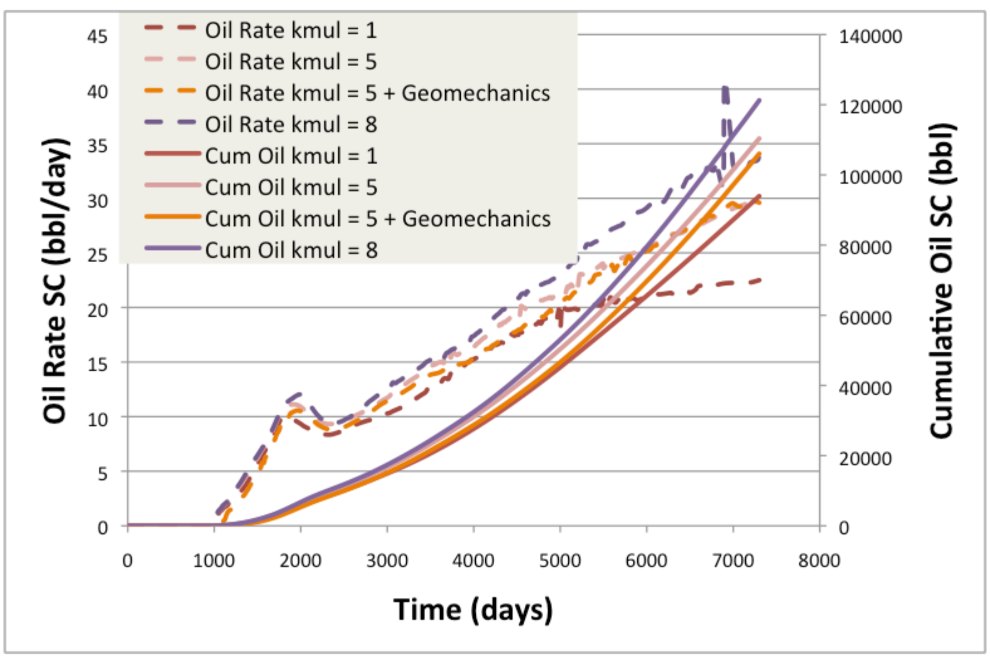


Figure 10: Sensitivity of predicted oil production from STARS simulations to the geomechanics module and to a parameter in Equation 1.

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

Subtask 4.3 researchers completed a milestone this quarter, the thermogravimetric analysis (TGA) experiments of oil shale utilizing fresh "standard" core. TGA experiments were completed at both atmospheric pressure and at 40 bar on small cores and on powdered samples by project team members at the University of Utah and Brigham Young University (BYU) as described below.

The Skyline 16 core was obtained to address some of the issues arising in analyzing data from aged samples. Three organic-rich (Mahogany zone) samples from the Skyline 16 core, all within a 90-foot depth (461.9 to 548.1 feet) interval were selected for experimentation: GR-1 (461.9- 462.9 feet), GR-2 (485.9- 486.9 feet), and GR-3 (548.1- 549.1 feet). In the previous quarterly report, Subtask 4.3 researchers summarized the TGA and CHNS (carbon, hydrogen, nitrogen and sulfur) data on powdered samples of GR-1, GR-2 and GR-3. Significant variation was found in terms of organic and elemental (CHNS) composition in these samples.

During this quarter, Subtask 4.3 researchers performed pyrolysis experiments and TGA analyses on samples from the GR-1, GR-2 and GR-3 sections that were 1 inch in diameter and approximately 6 inches long. For the pyrolysis tests, each core section was divided into three subsections. A 24-hour isothermal pyrolysis experiment was performed on each subsection (see Figure 11). High resolution Computer Tomography was also performed on these samples both before and after pyrolysis (see Subtask 4.5 summary).

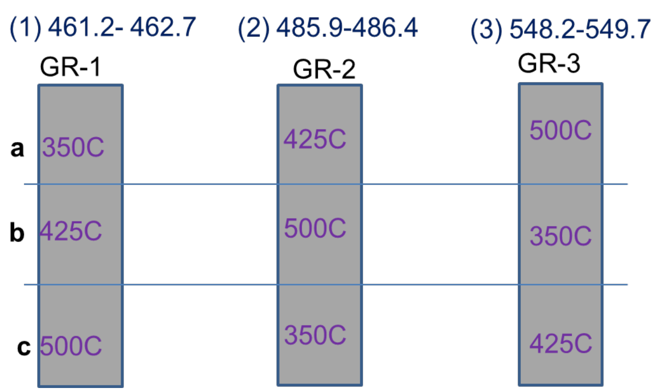


Figure 11: GR core sections that were subjected to isothermal pyrolysis at different temperatures for 24 hours. The cores were 1 inch in diameter and ~6 inches long.

Isothermal pyrolysis experiments were conducted for 24 hours with hot N_2 flow (~ 100 ml/min) from the top of the reactor. After pyrolysis, oil and gas samples were collected for compositional analyses. The weight loss and oil yield were measured and gas losses were calculated by difference. The results are summarized in Figure 12 and Table 2. In general, increased pyrolysis temperature increased the weight loss and oil yield. GR-1 is the richest organic sample and had more weight loss (and oil yield) compared to other samples.

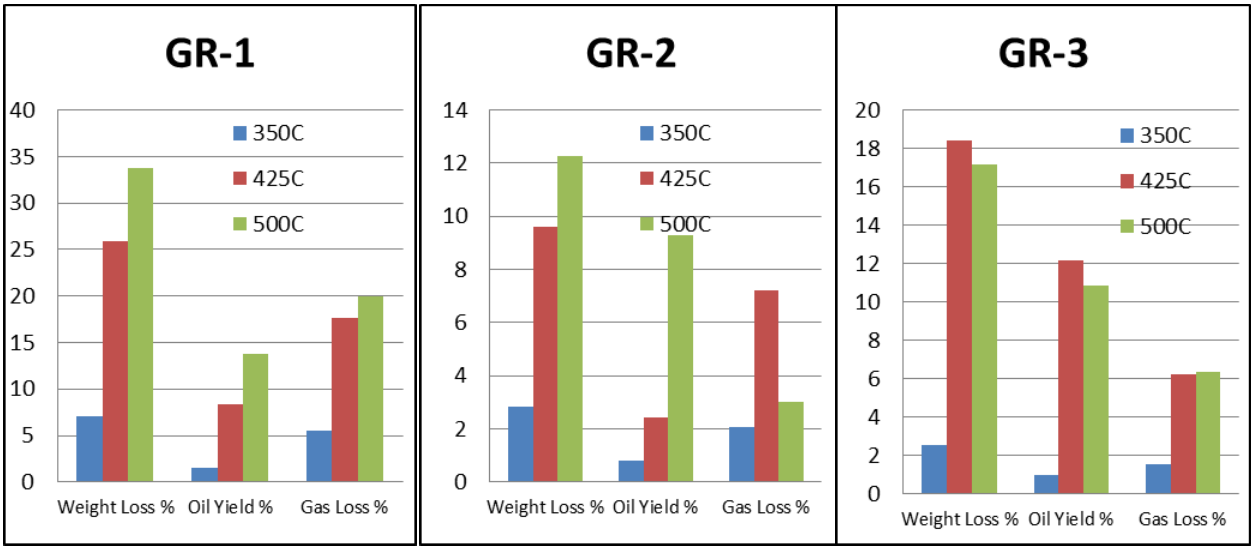


Figure 12: Results (weight loss %, oil yield % and gas loss %) from isothermal pyrolysis of GR core sections.

Table 2. Summary of results from GR core sample pyrolysis (reactor pyrolysis followed by TGA analysis of spent shales). The results are normalized based on initial weight.

Sample-ID		Reactor Pyrolysis					TGA pyrolysis and Combustion		
GR Core	ID	Initial weight, gm	Temp C	Weight Loss %	Oil Yield %	Gas Loss %	Unreacted Organic %	Mineral %	Coke %
GR-1	1a	40.32	350C	7.08	1.53	5.55	29.04	13.21	4.00
	1b	40.49	425C	25.91	8.31	17.60	31.21	7.92	3.15
	1C	41.63	500C	33.74	13.72	20.02	15.76	8.41	3.23
GR-2	2c	50.78	350C	2.84	0.79	2.05	13.92	27.04	0.14
	2a	61.82	425C	9.61	2.42	7.20	0.00	33.86	0.65
	2b	52.93	500C	12.26	9.27	2.99	0.00	23.53	0.10
GR-3	3b	51.75	350C	2.54	0.97	1.58	10.06	20.00	1.40
	3c	47.88	425C	18.40	12.15	6.25	0.00	24.36	4.41
	3a	51.20	500C	17.17	10.84	6.33	0.00	23.27	1.80

Images of the different subsections of spent shales after isothermal pyrolysis are shown in Figure 13. The core with highest organic content (GR-1) under high temperature (500°C) showed more deformation than lower temperature pyrolysis (350°C) samples and organic lean cores (GR-2). It was observed that 350°C was not adequate to obtain complete organic decomposition in 24 hours (less weight loss and correspondingly less oil yield).

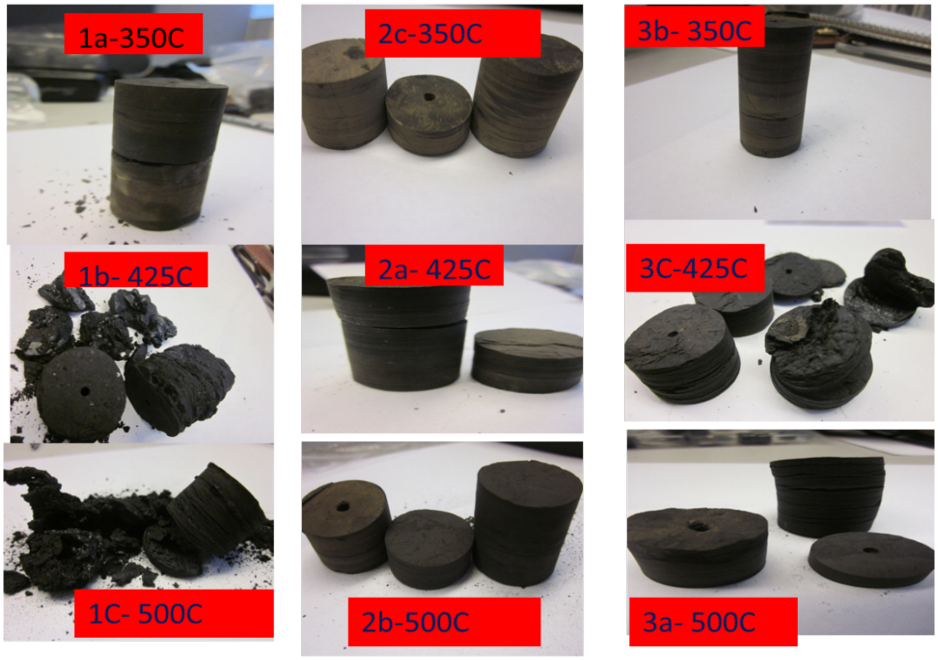


Figure 13: Images of the spent shales from GR core samples.

A small amount of each spent shale core was further pyrolyzed and combusted in a TGA to account for the unreacted organics remaining in the oil shale and the coke formed during the pyrolysis. Figure 14 shows a thermogram example of spent shale from GR-2. The results from the spent shale TGA analysis are summarized in Table 2. A significant amount of organic matter in GR-1 samples was left in the core either as unreacted organic matter or as heavy oil produced. GR-1 and the organic lean samples also produced more coke (GR-2 and GR-3).

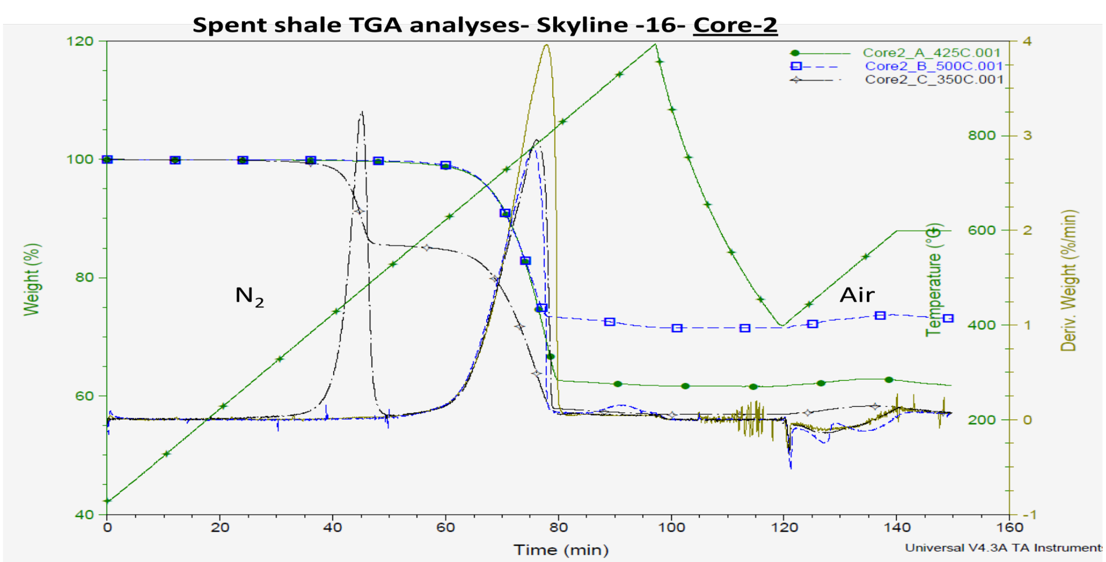


Figure 14: Thermogram of spent shale TGA analysis of GR-2. A combined pyrolysis (N_2) and combustion (air) TGA run was performed to account for unreacted organic and coke material in the spent shale.

The results from reactor pyrolysis are somewhat consistent with the TGA and CHNS analyses of the same sections. The GR-1 sample underwent large weight loss at the highest temperature, but, the oil yield does not correspond to weight loss (maximum of 13.7 % from GR-1). During high temperature isothermal pyrolysis, mineral decomposition may contribute to weight loss. The oil and gas samples collected are being analyzed using gas chromatography.

Also under Subtask 4.3, researchers at BYU collected TGA data for the GR-1, GR-2, and GR-3 powdered kerogen samples, began preliminary modeling of TGA data, tested demineralized kerogen samples from Subtask 4.9, and performed the initial set-up of the reactor to pyrolyze demineralized kerogen. To obtain the TGA data, approximately 10 mg of each powdered sample were heated to 850°C at one of three heating rates (1, 5, and 10 K/min) and one of two pressures (atmospheric pressure and 40 bar). Samples had a dwell time at 850°C of five minutes. This range of testing conditions resulted in six possible conditions for each sample and 18 unique experiments for the three samples, as shown in Table 3.

Table 3. Experimental conditions for each of the three samples.

	1 K/min	**5 K/min**	**10 K/min**
Atmospheric	X	X	X
40 bar	X	X	X

Characteristic TGA data are shown in Figure 15. The actual data are shown superimposed on the smoothed data. Flow rates of helium were kept constant for all runs in order to minimize randomizing factors. As expected, two separate reactions are observed in Figure 15. At atmospheric pressure, the kerogen pyrolyzes at approximately 450°C and the calcium carbonate at 650°C. The project team is in the process of reducing the TGA data; separate kinetic coefficients will be determined for each sample at each pressure. Once the data are reduced to eliminate noise and the effects of buoyancy, the data will be fit with a first-order reaction rate expression following the method of Hillier et al. (Hillier et al., 2010; Hillier and Fletcher, 2011). Previously, Subtask 4.3 researchers have shown that the temperature where pyrolysis occurs increases slightly with elevated pressure (Hillier et al., 2010; Hillier, 2011; Hillier and Fletcher, 2011).

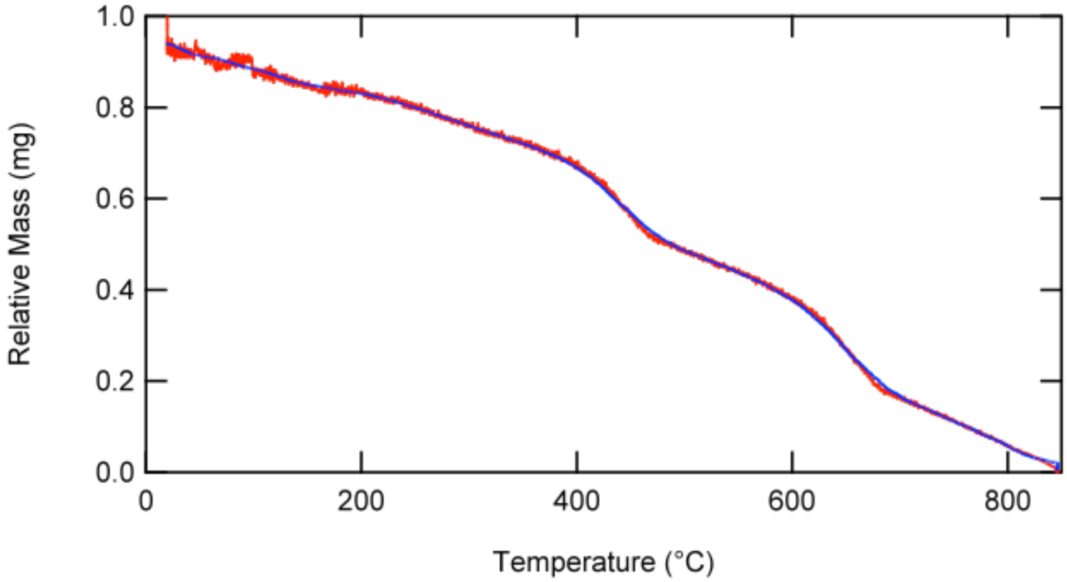


Figure 15: GR1RAW sample at 10K/min and 1 atm.

Figure 16 shows an example of how buoyancy curves will be used to analyze the data. Curves are extrapolated from regions where the sample is not reacting in order to subtract buoyancy effects. The sample is removed from the TGA and weighed at the end of the experiment. The final corrected mass is checked against the final measured mass for consistency.

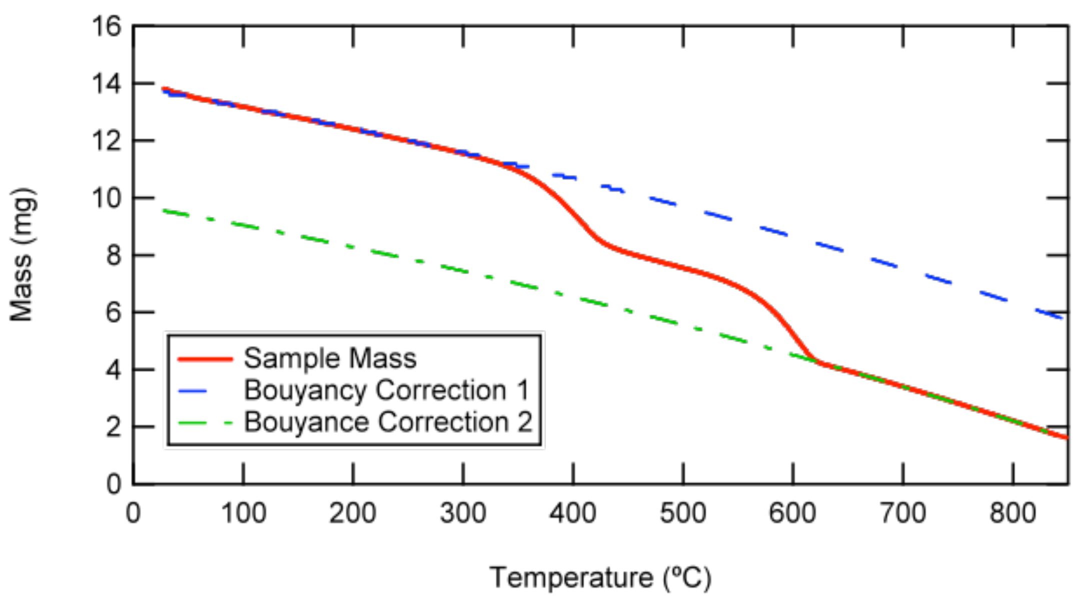


Figure 16: Method to correct for buoyancy; adapted from (Hillier, 2011).

Subtask 4.3 researchers have also been working with researchers in Subtask 4.9 to optimize the demineralization process. The initial sample of demineralized kerogen received from Subtask 4.9 contained a large amount of ash (see Subtask 4.9 summary below). Researchers from both tasks worked together to perform nine separate ash tests on varying samples of demineralization kerogen until an acceptable process was found. Different methods included use of hydrochloric, fluoric, and/or boric acid combined with other techniques. Each sample was tested according to the ASTM ashing process, which requires the sample to be heated in a furnace at a steady rate to 750°C and held at that temperature for 10 hours. On a dry basis, sample ash percent ranged from 70% in primary samples to 5% in the final sample, labeled GR1.9. The first ash test (70% ash content) was evaluated using a scanning electron microscope (SEM) to determine the components of remaining ash, which turned out to be mostly calcium. The SEM was moved shortly after that first test, so further ash evaluation was not possible.

About seven grams of sample GR1.9 demineralized kerogen was recently received from Subtask 4.9 researchers for pyrolysis in the kerogen retort. The kerogen retort had to be reassembled for these pyrolysis experiments. The purpose of the retort experiments is to generate char and "tar" samples to analyze chemically with the NMR techniques at the University of Utah. A schematic of the kerogen retort is shown in Figure 17. One gram of sample will be used for each experiment; the heating rate is 10 K/min. The furnace used to heat the reactor apparatus was repaired and all other preparations were completed prior to the pyrolysis experiments. These tests will commence during the first week of November.

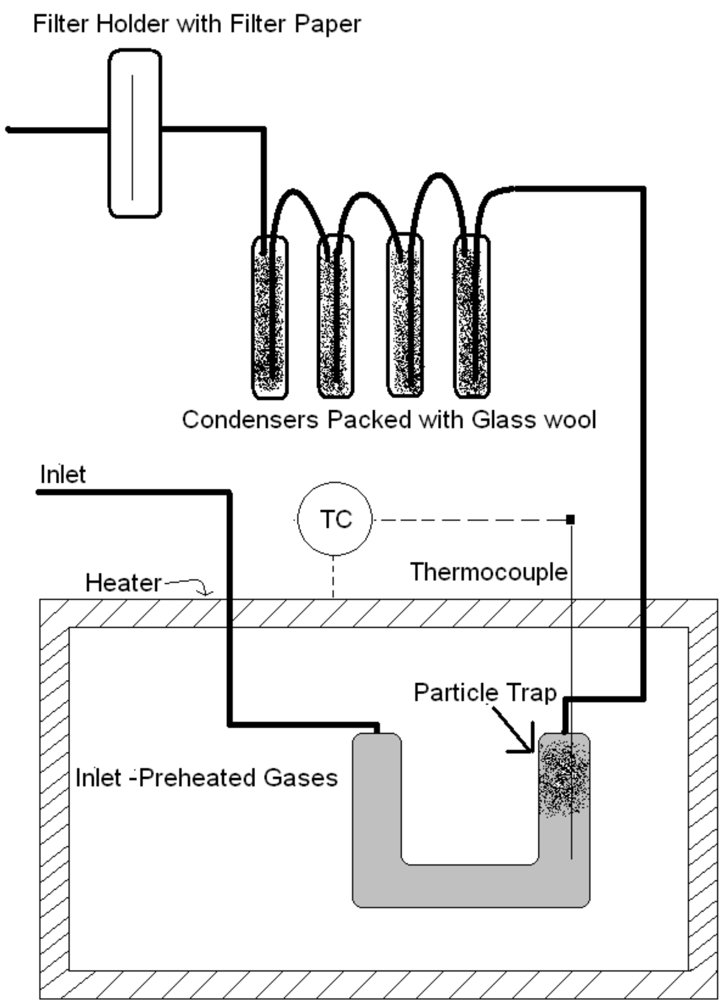


Figure 17: Schematic of the kerogen retort.

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

This project has been completed.

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

Research in Subtask 4.5 is focused on understanding pore scale transport processes in the pyrolysis of oil sand and oil shale using 3D multiscale X-ray computed tomography (CT) analysis coupled with Lattice Boltzmann (LB) simulation. Research performed during this quarter involved Skyline 16 oil shale cores. Three fresh Skyline 16 oil shale cores (6 inches long, 1 foot in diameter), located from 461.2-461.7 feet (core 1), 485.9-486.4 feet (core 2), and 548.2-548.7 feet (core 3), were provided by Subtask 4.3 researchers group. Four sections (1 – 4 from top to bottom) were scanned independently to complete the full-length 3D image of each core prior to pyrolysis.

The 3D volume rendered images from the reconstructed x-ray CT data (~42 micron voxel resolution) for the three Skyline 16 oil shale drill core samples (three cores, 4 scans per core) are shown in Figures 18, 19, and 20.

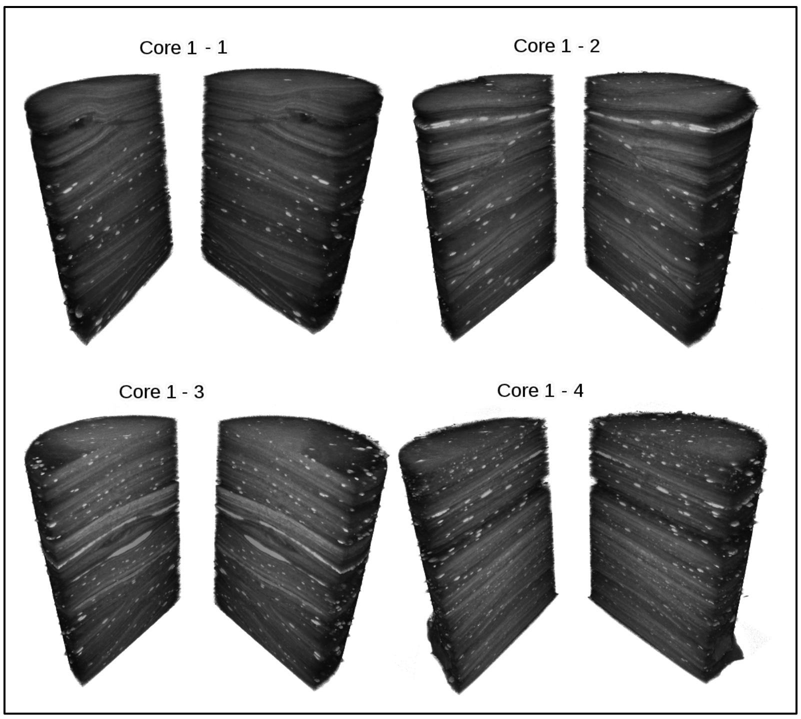


Figure 18: 3D volume rendered images from reconstructed x-ray CT data for core 1; ~42 micron voxel resolution. Core scanned in four sections.

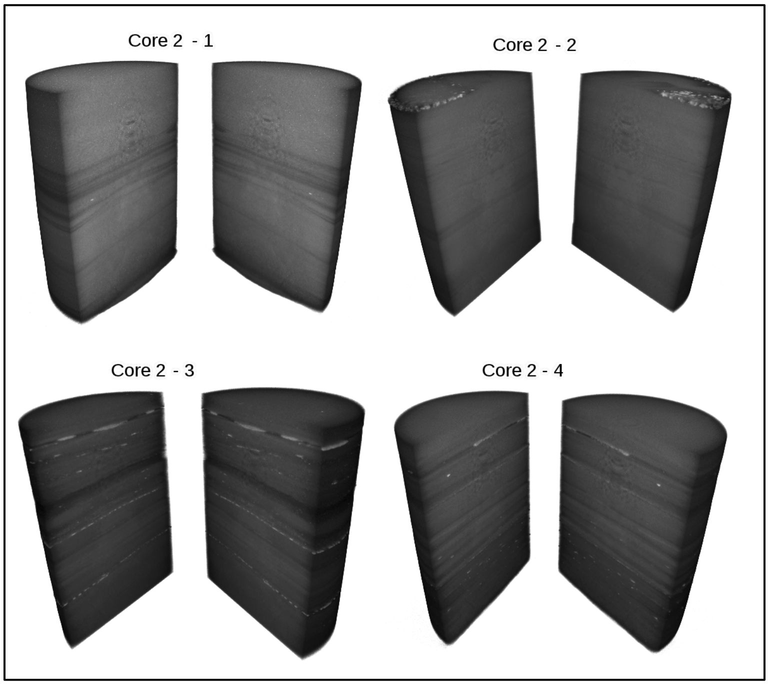


Figure 19: 3D volume rendered images from reconstructed x-ray CT data for core 2; ~42 micron voxel resolution. Core scanned in four sections.

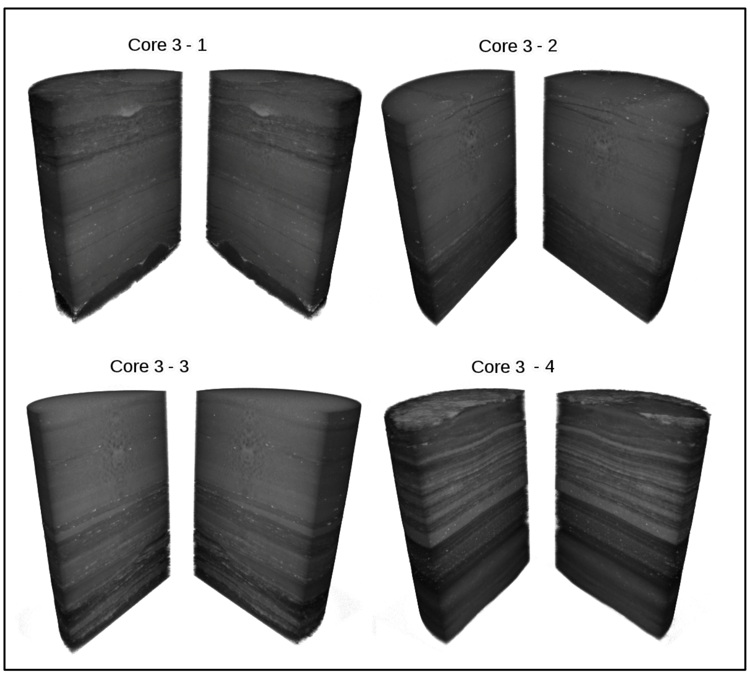


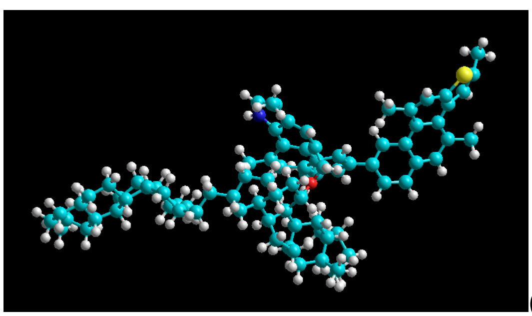
Figure 20: 3D volume rendered images from reconstructed x-ray CT data for core 3; ~42 micron voxel resolution. Core scanned in four sections.

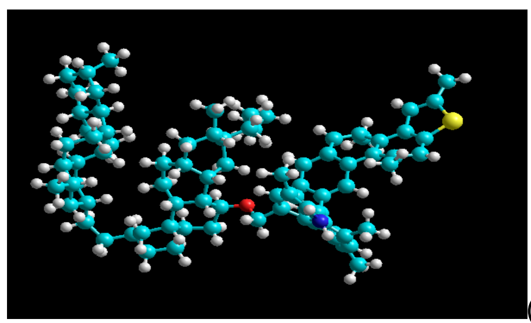
Future research will identify critical fundamental factors of pore geometry and structure which limit recovery of hydrocarbons from oil sand and oil shale.

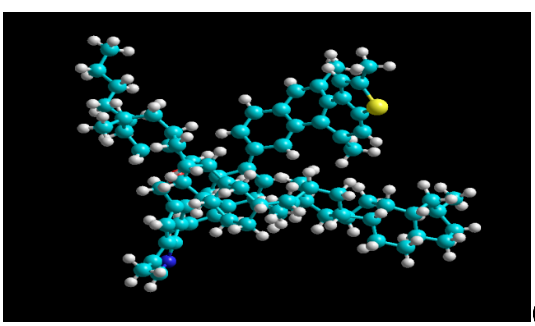
Subtask 4.6 - Atomistic Modeling of Oil Shale Kerogens and Oil Sand Asphaltenes (PI: Julio Facelli)

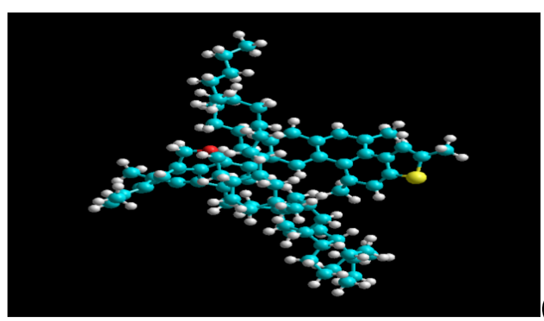
In this quarter, Subtask 4.6 researchers developed optimized 3D structures for the mid-continent asphaltene, based on the 2D model proposed by Siskin et al. (2006). They first attempted to scan the dihedral angles between the aliphatic and aromatic parts of the structure by using the routines available in the Gaussian set of programs. However, this process was very time consuming and thus impractical. Next, they selected 216 configurations of the model for the midcontinent asphaltene by systematically varying the three dihedral angles formed between the aliphatic and the aromatic parts of the model. Keeping the dihedral angles fixed for each of those 216 configurations, the optimized the structures using density functional theory. Out of 216 configurations, only 56 converged to valid optimized geometries. The energy of the optimized geometries and the corresponding distances between aliphatic and aromatic parts of these different configurations were then analyzed. The project team concluded that it is difficult to find a rule for choosing representative structures on which to perform further calculations testing the sensitivity of ^{13}C nuclear magnetic resonance (NMR) spectra to molecule configuration.

In order to test the sensitivity of ^{13}C NMR spectra to the configuration of the asphaltene molecule, Subtask 4.6 researchers generated eight different geometrical configurations of single units of mid-continent asphaltene using molecular mechanics. In the molecular mechanics simulations, researchers used the MM+ force field as implemented by the program HyperChem. Keeping a single unit of the midcontinent asphaltene in a cubical box of dimension 30 Å × 30 Å × 30 Å , the system was heated and annealed at different conditions by varying the temperature and the simulation time. The eight different configurations obtained by simulated annealing are shown in Figure 21.


(a)


(b)


(c)


(d)

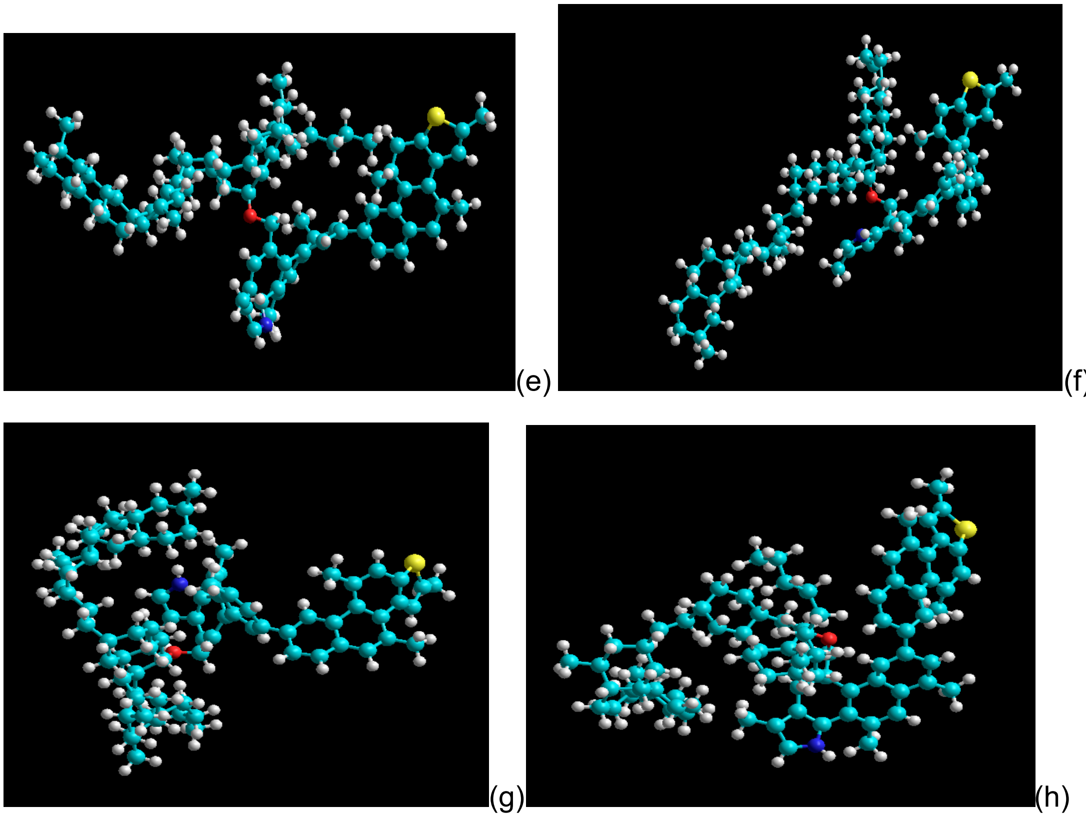
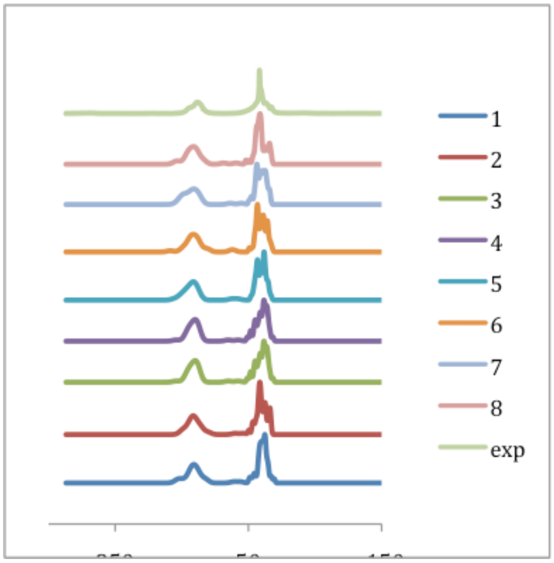
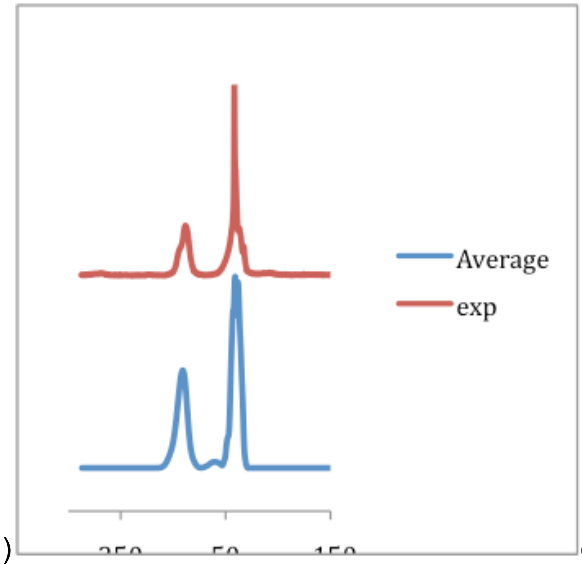


Figure 21. Eight different structures obtained by simulated annealing of a single unit of midcontinent asphaltene.

The ^{13}C NMR spectra for these eight different structures are presented in Figure 22. The calculations of the NMR chemical shifts were performed with the 3-21G basis set as implemented in the Gaussian set of programs. After the calculations of the chemical shifts, the NMR spectra was calculated by adding a Gaussian broadening to the chemical shifts of all the carbons in the model. For comparison, the experimental NMR plot from Siskin et al. (2006) is also included in the figure. From Figure 22, it is clear that the NMR spectra for different configurations are slightly different, which shows that the NMR spectrum is sensitive to the configuration of asphaltene units. The average spectra of these eight structures is also shown in Figure 22.

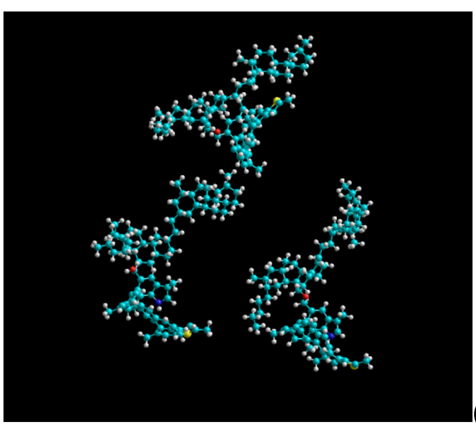
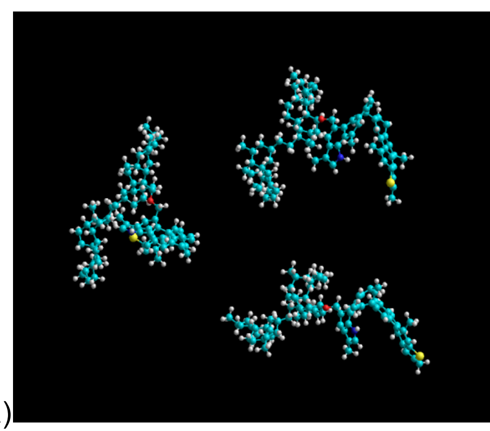


(a)


(b)

Figure 22: (a) ^{13}C NMR spectra for the eight different configurations of single unit of midcontinent asphaltene obtained by simulated annealing, (b) ^{13}C NMR spectra for average of configurations from (a).

To explore the importance of stacking on the ^{13}C NMR spectra of mid-continent asphaltene, Subtask 4.6 researchers placed three units of the mid-continent asphaltene in a 50Å×50Å×50Å box and performed a similar simulated annealing procedure as for the single units. The resulting five structures are shown in Figure 23. The corresponding NMR spectra of all eight structures and their average are shown in Figure 24. As found with the single units, the spectra are quite sensitive to the configuration of the stacks. The energies for the different configurations for the single unit and the stack models obtained by the molecular mechanics method are presented in Table 4.


(a)

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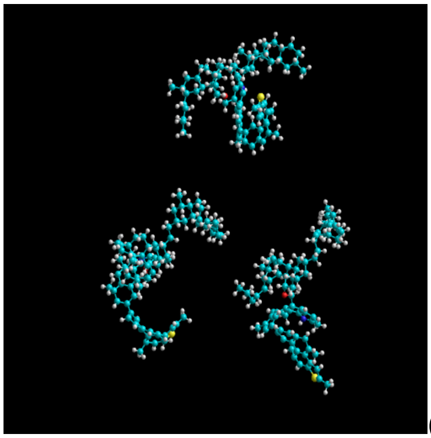
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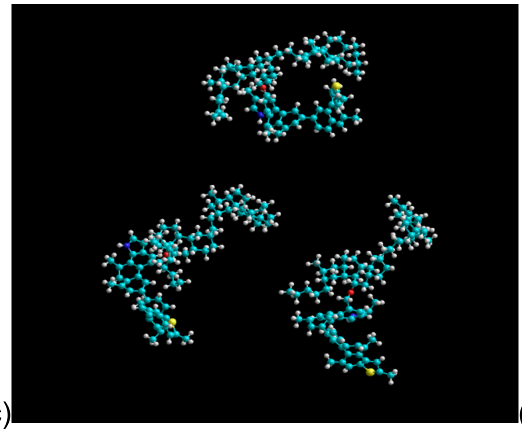
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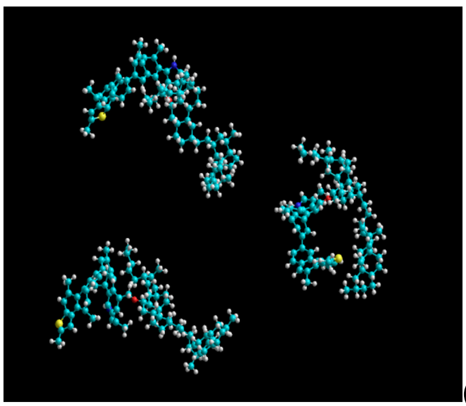
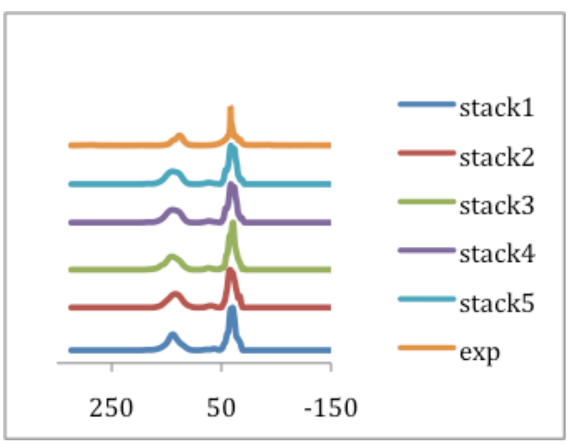
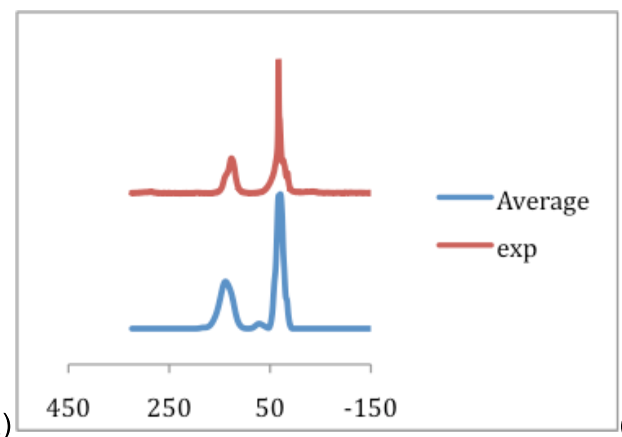

(e)

Figure 23: Five different structures obtained by simulated annealing of the stack of three units of midcontinent asphaltene**.**



(a)


(b)

Figure 24: (a) ^{13}C NMR spectra for the five different configurations of trimmers of mid-continent asphaltene obtained by simulated annealing, (b) ^{13}C NMR spectra for average of configurations from (a).

Table 4. Energies for the different configurations for the single unit and the stack models obtained by molecular mechanics method.

Single unit	**Kcal/mol**
Conf.1	384.7232
Conf. 2	379.6681
Conf. 3	377.8388
Conf. 4	377.8729
Conf. 5	370.4313
Conf. 6	393.7743
Conf. 7	371.8277
Conf. 8	423.615
Stack of three units	**Kcal/mol**
Conf. 1	1135.171
Conf. 2	1070.918
Conf. 3	1133.462
Conf. 4	1081.728
Conf. 5	1081.728

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

The Subtask 4.7 research team completed a milestone during this quarter; the pressure vessel has been fabricated and pressure tested and the ancillary flow system is being designed and modified. Additionally, a prototype copper jacket was fabricated in the machine shop. This jacket is a very thin-walled copper tube that will prevent confining fluid (nitrogen) from entering the sample during testing. The copper tubing has been milled down to a thickness of 0.010 inches for this purpose. Team members also consulted with a mechanical engineering specialist (R. Nielson at TerraTek, Inc.) on the design of sample end caps. Based on the specialist's recommendations, the Subtask 4.7 team has redesigned the sample end caps and has begun to take inventory of components to provide the axial loading and to collect samples downstream of the core being tested and outside of the vessel.

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

Subtask 4.8 researchers have completed drafting the sedimentary log of the Skyline 16 core. This core log will be distributed to researchers in other tasks and subtasks. X-ray fluorescence (XRF) analysis has been performed on 153 samples from the Skyline 16 core to delineate stratigraphic changes in elemental composition, which will be used as a proxy for mineralogic composition. QEMscan analysis has also been completed on the five samples listed below from the Skyline 16 core:

GR-1 - 461.93-462.92 - Mahogany rich
GR-2 - 485.9-486.94 - Mahogany lean
GR-3 - 548.18-549.15 - Upper R-6 rich
GR-4 - 410.4-410.5 - R-8 rich

GR-5 - 812.15-812.3 - R-5 rich

Detailed mineralogic data from QEMScan analysis can be mapped/imaged and analyzed quantitatively/statistically.

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

Last quarter, Subtask 4.9 researchers reported that they had isolated kerogen from 100 mesh ground shale of the three previously identified segments of the Skyline 16 core (GR-1, GR-2, GR-3) following the process outlined by Vandergrift et al. (1980). Researchers also completed the NMR analysis on these samples and obtained small angle X-ray scattering (SAXS) and PDF measurements at the Advanced Photon Source (APS) at Argonne National Laboratory (ANL). The initial nuclear magnetic resonance (NMR) spectra gave the appearance that the demineralization was successful, but the PDF analysis completed at ANL indicated that there was still a high concentration of mineral matter in the samples. Subsequent to this, the samples were sent for ash testing; this test confirmed that a large amount of mineral matter was still present in the samples.

This finding led to the exploration of options for the removal of the remaining mineral matter. It was found that doing a final hydrochloric acid/boric acid wash followed by another hydrochloric acid wash gave a clean sample. Ashing tests on a GR-1 sample with the additional treatments confirmed a mineral content of approximately 5%. These additional steps were completed on both the GR-1 and GR-2 samples. A small amount of both samples underwent SEM/EDX analysis which confirmed a very low mineral content. The NMR experiments were repeated on these clean samples. Following the procedure outlined by Solum et al. (1989), the spectra obtained along with the results of the analysis are shown in Figure 25. Table 5 list results obtained on samples in this quarter as well the analyses of the three shale samples previously completed.

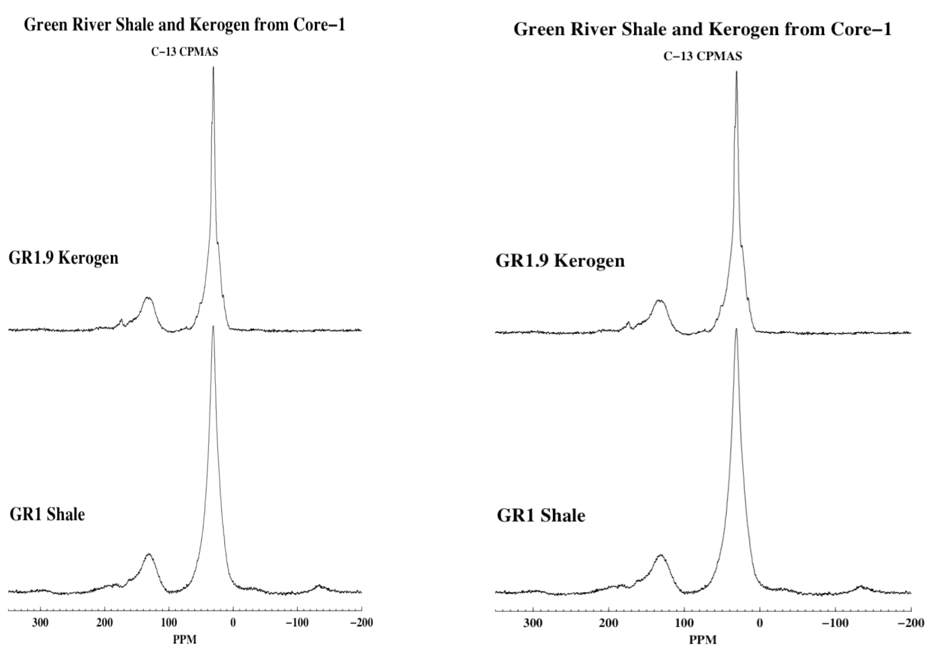


Figure 25: ^{13}C NMR CP/MAS spectra from GR-1 and GR-2 raw shale and isolated kerogen samples.

Table 5. Structural and lattice parameters for the GR-1, GR-2, and GR-3 kerogens (after Solum et al., 1989).

Green River Shales and Their Kerogens from Three Cores[1,2]

Structural Parameters

Compound	f_a	f_a^C	f_a^O	f_a^{OO}	$f_{a'}$	f_a^H	f_a^N	f_a^P	f_a^S	f_a^B	f_{al}	f_{al}^H	f_{al}^*	f_{al}^O
Gr1 (CP) cr	0.25	0.04	0.02	0.02	0.21	0.07	0.14	0.04	0.07	0.03	0.75	0.62	0.13	0.02
Gr1.9 (CP)	0.24	0.04	0.01	0.03	0.20	0.06	0.14	0.03	0.07	0.04	0.76	0.65	0.11	0.00
Gr2 (CP) nc	0.22	0.04	0.02	0.02	0.18	0.06	0.12	0.03	0.06	0.03	0.78	0.65	0.13	0.00
Gr2.9 (CP)	0.23	0.05	0.02	0.03	0.18	0.06	0.12	0.03	0.06	0.03	0.77	0.66	0.11	0.01
Gr3 (CP) cr	0.34	0.06	0.04	0.02	0.28	0.08	0.20	0.04	0.09	0.07	0.66	0.52	0.14	0.03
Gr3.9 (CP)														

Lattice Parameters

Compound	χ_b	C	$\sigma+1$	P_0	$B.L.$	$S.C.$	$M.W.$	M_δ
Gr1 (CP)	0.143	8.4	4.4	-0.18	--	--	--	--
Gr1.9 (CP)	0.200	10.0	5.0	-0.10	--	--	--	--
Gr2 (CP)	0.167	9.0	4.5	-0.44	--	--	--	--
Gr2.9 (CP)	0.167	9.0	4.5	-0.22	--	--	--	--
Gr3 (CP)	0.241	11.6	5.6	-0.08	--	--	--	--
Gr3.9 (CP)								

1. cr - corrected for large aliphatic sidebands due to ferrimagnetic particles in raw shale.
2. nc – not corrected for very small aliphatic sidebands due to ferrimagnetic pparticles in raw shale

In addition to C-13 NMR, some preliminary Si-29 NMR was completed on the shales to see if there were any measurable differences in the silicon of the mineral matter/clay. Silicon chemical shifts of silicates and aluminosilicates are very distinctive depending on bonding arrangement about the silicon, which are classified as Q^0 – Q^4 (Lippmaa et al., 1980). Figure 26 shows that there are distinct differences between GR-1, GR-2, and GR-3, especially in the amount of Q4 type silicons (Si with 4 O-Si groups). Further analysis will be needed to see if silicon NMR can be used to gain insight into the structure of the clay.

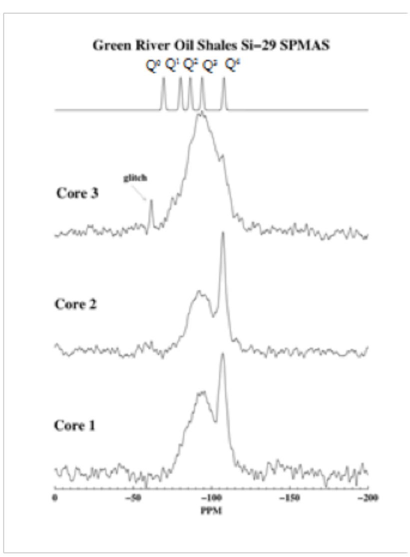


Figure 26: SI-29 NMR spectra from GR-1, GR-2, and GR-3 raw shale samples.

Finally, the analysis for pore size distribution was started on the SAXS measurements from the raw shales; the data obtained on the kerogens will need to be retaken on the clean (e.g. demineralized) samples. This analysis required first learning the analysis software, a package called IGOR, used in conjunction with a set of SAXS analysis modules developed at the APS. Figure 27 shows the SAXS scattering curves obtained for the ground shales of all three GR samples. On these scattering curves, the results of power law fits are also shown. The exponent of the three fits is between 3 and 4, consistent with that found for other shales. This exponent is related to the fractal dimension (6-exp = fractal dimension), a term dependent on the smoothness of the surface of the measured feature. If the exponent was 4, the surface is smooth; as the exponent decreases, fractal dimension increases, meaning the surface has folds and is very convoluted. The analysis of the remaining SAXS data on both the whole rock and ground shale will be continued.

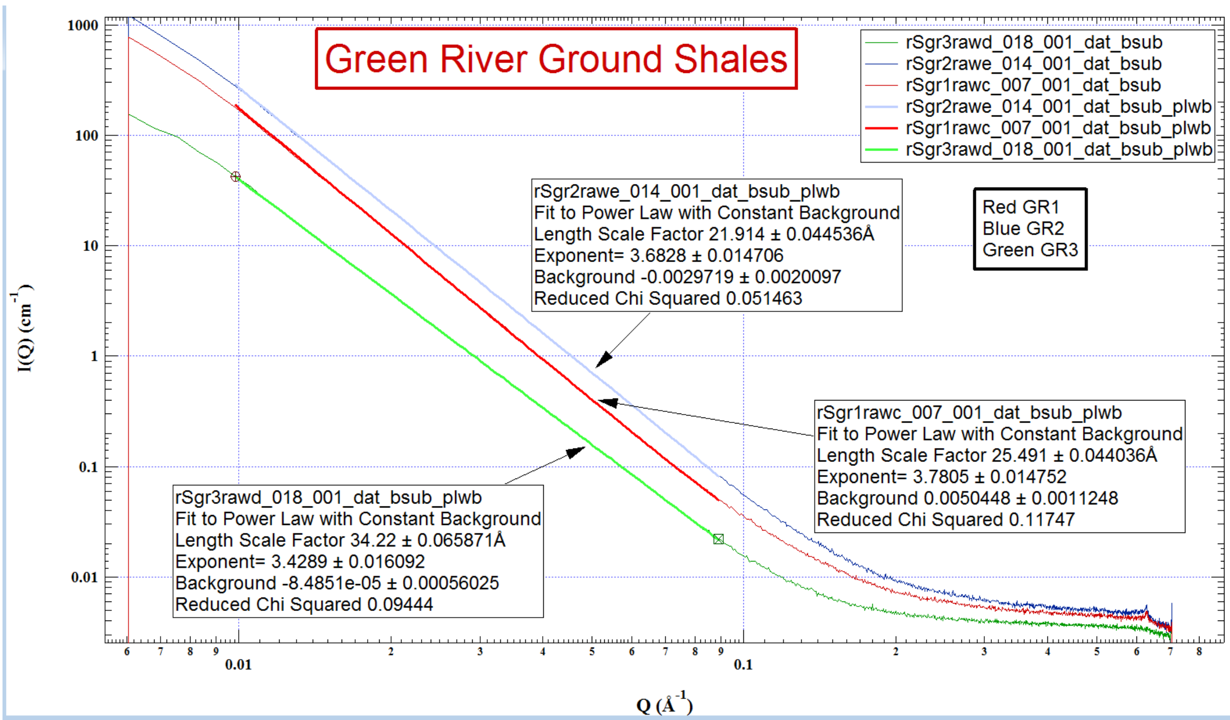


Figure 27: SAXS scattering curves obtained from GR-1, GR-2, and GR-3 raw shale samples.

An additional analysis which gives the pore diameter, the Guinier Fit, was completed on the SAXS curves of these three samples. The Guinier analysis for GR-3 is shown in Figure 28. The pore diameter was determined to be 3.2 Å, consistent with those measured for GR-1 and GR-2.

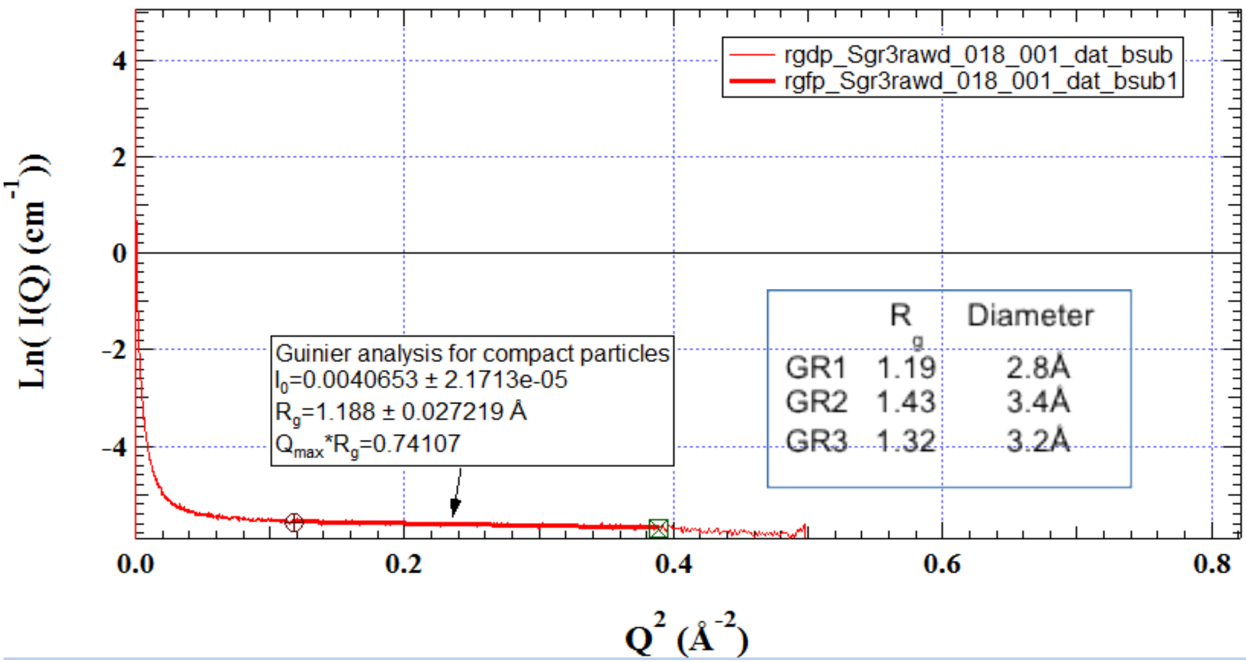


Figure 28: Pore diameter for GR-3 raw oil shale samples from Guinier analysis.

Finally, samples of both the GR-1 and GR-2 kerogens were sent to ANL for new PDF measurements. The PDF obtained for GR-1 will provide the data needed to complete the paper entitled "*Three-Dimensional Structure of the Siskin Green River Oil Shale Kerogen Model: A Computational Study*" by Pimienta, Orendt, Pugmire, Facelli, Locke, Winans, Chapman and Chupas.

Task 5.0 - Environmental, Legal, Economic and Policy Framework

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

A Subtask 5.1 milestone was completed last quarter but mistakenly omitted from the discussion of Subtask 5.1 in the April-June 2011 quarterly report. The milestone was to identify case studies for the assessment of multi-jurisdictional resource management models and to evaluate the utility of those models in context of oil shale and sands development. The models selected for discussion in the Subtask 5.1 topical report are: Project Bold; the Utah Schools and Lands Improvement Act of 1993; creation of the Grand Staircase-Escalante National Monument; the GSENM Land Exchange; the Utah West Desert Land Exchange; the San Rafael Swell Land Exchange; the Cedar Mountain Wilderness; the Utah Recreational Land Exchange; the Uintah and Ouray Indian Reservation Exchange; the Washington County Growth and Conservation Act; the Red Rocks Wilderness Bill; and Wild Lands.

Subtask 5.1 researchers attended the 2011 Energy Forum, a Stegner Center workshop on energy issues, a meeting of the Bureau of Land Management's Resource Advisory Committee, and meetings of the Natural Resources, Agriculture, and Environment Interim Committee. Project team members met informally with staff from the Bureau of Land Management, the Department of Wildlife Resources, the School and Institutional Trust Lands Administration, the Governor's Public Lands Policy Coordination Office, and the Division of Forestry, Fire, and State

Lands, as well as the new State Alternative Energy Development Manager. Researchers also met informally with attorneys representing the State of Utah and energy industry clients and with members of the environmental community. These meetings provided broad perspectives on public land management, barriers to cooperation, and potential strategies to facilitate more effective management. Subtask 5.1 researchers continued to track the Department of the Interior's evolving policies regarding management of wilderness quality public lands, relevant federal and state legislative responses, and associated litigation. Researchers continued drafting portions of the topical report examining issues associated with wilderness quality land management, its implications for unconventional fuel developers, and potential paths forward. Subtask 5.1 researchers finalized mapping and quantification of wilderness quality lands within Utah that may impact oil shale and oil sands development.

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

This quarter, Subtask 5.2 researchers completed the milestone of completing "research on conjunctive surface water and groundwater management in Utah, gaps in its regulation, and lessons that can be learned from existing conjunctive water management programs in other states." Subtask 5.2 researchers also worked on drafting and editing topical report sections addressing the management framework for hydraulically connected surface and groundwater within Utah, conjunctive management of surface and groundwater resources in neighboring states, and conjunctive surface and groundwater management's implications for unconventional energy developers. Researchers also continue to monitor the State's Executive Water Rights Taskforce and Interim Natural Resources, Agriculture, and Environment Committee for legislative proposals likely to impact conjunctive water resource management within Utah.

During this quarter, Subtask 5.2 researchers attended the Salt Lake County Watershed Symposium and meetings regarding environmental review of proposals to develop groundwater underlying the Utah-Nevada border. Researchers met informally with staff from the Utah Department of Wildlife Resources, the Governor's Public Lands Policy Coordination Office, and the Division of Forestry, Fire, and State Lands, as well as the new State Alternative Energy Development Manager. Project team members also met informally with attorneys representing the State of Utah and other water users and members of the environmental community. These meetings provided insights into practical conjunctive water resource management efforts as well as emerging issues of concern resulting from conjunctive management project development.

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

No report received.

6.0 – Economic and Policy Assessment of Domestic Unconventional Fuels Industry

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

During this quarter, the Subtask 6.1 team worked to finalize the details of the four unconventional fuel development scenarios in Utah's Uinta Basin. The ex situ oil shale scenario includes an underground mine, a surface retort employing a TOSCO II retorting technology, and an upgrading facility to remove nitrogen and sulfur. This scenario has been reviewed with an oil shale industry consultant, Mr. Bob Loucks. The in situ oil shale scenario was difficult to develop as no technologies currently exist that could be directly applied. Because of the cost and inefficiency of electrical heating, the project team determined that no large-scale production would be attempted using conductive heating from electrical resistance heaters. Instead, team members proposed direct-fired heaters as the most efficient way to deliver a desired heat flux to kerogen-rich underground resources. Radiant heaters were selected as the technology of choice and potential costs were determined from research papers and industry literature. The uncertainty bands on the supply costs for this scenario are very large due to the speculative nature of the technology. Costs for both oil shale scenarios are determined based on a production capacity of 50,000 barrels of oil per day (BOPD). The size of the potential oil sands production was reduced from 50,000 BOPD to 10,000 BOPD due to the intermittent nature of the various oil sands deposits and the lack of detailed information on resource quality and quantity. The ex situ oil sands scenario includes a surface mine, a solvent-based extraction process similar to that proposed by a company pursuing oil sands development in the Uinta Basin, and both primary and secondary upgrading steps. The technology employed for the in situ oil sands scenario is not speculative; steam-assisted gravity drainage is the technology of choice in Alberta for in situ production of Athabasca oil sands. What is speculative is the assumption that the quality of the resource could support a 10,000 BOPD operation. Lack of available data on resource quality makes the error bars on the supply costs for this scenario very wide. The project team is currently determining final supply cost numbers for all four scenarios for inclusion in the Market Assessment (see Subtask 6.3).

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

During this quarter, Subtask 6.2 researchers continued to review and edit the economic analysis contrasting Canadian oil sands development and potential domestic oil sands development. The topical report being prepared for this Subtask was to have been completed during this quarter but has been delayed due to continuing revisions and drafting required both by reviewer comments and the need for analytic consistency between the economic analysis of oil sands presented in the topical report for this Subtask and the Market Assessment report. Completion of the topical report for this Subtask is expected by the end of the next quarter.

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

Subtask 6.3 researchers made significant revisions based on reviewer comments. Entire sections have been rearranged and/or rewritten. Due to intense interest from the media in the numbers that will be published in this assessment, researchers are still carefully reviewing all assumptions, methodologies, reporting protocols, and sources. This process has taken longer than anticipated, delaying release of the final draft. The project team is currently on track to release the final draft by the end of November 2011.

7.0 – Strategic Alliance Reserve

The intent of the Strategic Alliance Reserve was to fund collaborative projects with industry that built on ICSE research of the past years to move technologies closer to deployment. In the previous quarter, the milestone to complete the review and selection of SAR applications was accomplished but not noted in the quarterly report. A second milestone was completed during this quarter. The milestone was to implement new SAR research tasks; its completion is discussed next.

The Task 7.0 project team worked with an industrial collaborator, American Shale Oil (AMSO), to finalize a Statement of Project Objectives (SOPO), project budgets, and project timelines. Three new subtasks will be funded from the Strategic Alliance Reserve. These subtasks are:

- Geomechanical model - This research proposes the development of non-linear stress-strain relationships for oil shale with specific reference to AMSO properties. This constitutive model will need to capture the effects of temperature, the in-situ stress tensor, and the rate of mechanical or thermal loading on the incremental change in porosity (volume and saturation/infill), tangential values of Young's moduli, and Poisson's ratios and post-peak performance.
- Kinetic compositional models and thermal reservoir simulators - The objective of this task is to package the kinetic compositional model so that it can be incorporated into simulators at the University of Utah (and elsewhere) and to enhance the efficiency and physical rigor of the the reservoir-based simulator to more realistically represent all the complex processes during oil shale pyrolysis and subsequent production of multiple phases.
- Rubblized bed high performance computing simulations - This task's objective is to use a multiscale, multiphysics, high performance computer simulator to compute the behavior of the rubblized bed in the AMSO test by resolving the scale of the individual rubblized pieces of shale. Specifically, researchers intend to accurately predict the time/temperature history of each piece of shale in a statistical distribution of rubble in the AMSO configuration.

A fourth project involving burner testing is being funded separately by AMSO. An updated SOPO and Project Management Plan that includes these three subtasks will be submitted for approval in the next quarter; progress reports on these subtasks will subsequently be added to the quarterly report.

CONCLUSIONS

The Clean and Secure Energy from Domestic Oil Shale and Oil Sands Resources program is now fully implemented with the completion of the SOPO for the three projects being funded with money from the Strategic Alliance Reserve. One FY2010 project, Subtask 5.3, has yet to be initiated as researchers are still working on completion of Phase I deliverables for Subtask 6.2. Other projects from Phase I with deliverables that still need to be completed include Subtask 3.1, 3.2, 6.1, and 6.3. These projects should all be wrapped up in the next quarter.

COST STATUS

COST PLAN/STATUS

Baseline Reporting Quarter - PHASE I	Yr. 1								Yr. 2			
	Q1		Q2		Q3		Q4		Q5		Q6	
	7/1/09 - 12/31/09		1/1/10 - 3/31/10		4/1/10 - 6/30/10		7/1/10 - 9/30/10		10/1/10 - 12/31/10		1/1/11 - 3/31/11	
	Q1	**Total**	Q2	**Total**	Q3	**Total**	Q4	**Total**	Q5	**Total**	Q6	**Total**
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	449,459	**3,078,729**	314,813	**3,393,542**		**3,393,542**		**3,393,542**		**3,393,542**		**3,393,542**
Non-Federal Share	48,902	**699,537**	48,835	**748,372**		**748,372**		**748,372**		**748,372**		**748,372**
Total Incurred Costs	498,361	**3,778,266**	363,648	**4,141,914**		**4,141,914**		**4,141,914**		**4,141,914**		**4,141,914**
Variance												
Federal Share	262,926	**694,297**	312,610	**1,006,907**		**1,154,358**		**1,301,809**		**1,449,260**		**1,694,707**
Non-Federal Share	129,198	**243,972**	108,019	**351,991**		**388,854**		**425,717**		**462,580**		**521,486**
Total Variance	392,124	**938,269**	420,629	**1,358,898**		**1,543,212**		**1,727,526**		**1,911,840**		**2,216,193**

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			
2.0	Technology Transfer and Outreach			
	Advisory board meeting	Jun-12		
	Hold final project review meeting in format determined jointly by DOE/NETL and ICSE	Jun-13		
3.0	Clean Oil Shale & Oil Sands Utilization with CO2 Management			
3.1	Lifecycle greenhouse gas analysis of conventional oil & gas development in the Uinta Basin			
	Complete modules in $CLEAR_{uff}$ for life-cycle CO2 emissions from conventional oil & gas development in the Uinta Basin	Jun-12		
3.2	Flameless oxy-gas process heaters for efficient CO2 capture			
	Preliminary report detailing results of skeletal validation/uncertainty quantification analysis of oxy-gas combustion system	Oct-11		
3.3	Development of oil & gas production modules for $CLEAR_{uff}$			
	Develop preliminary modules in $CLEAR_{uff}$ for conventional oil & gas development & produced water management in Uinta Basin	Oct-11		
3.4	V/UQ analysis of basin scale $CLEAR_{uff}$ assessment tool			
	Develop a first generation methodology for doing V/UQ analysis	Oct-11		
	Demonstrate full functionality (integration of all modules) of V/UQ methodology for conventional oil & gas development in Uinta Basin	Apr-12		
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			

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

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

ID	Title/Description	Planned Completion Date	Actual Completion Date	Milestone Status
7.0	Strategic Alliance Reserve			
	Conduct initial screening of proposed Strategic Alliance applications	Mar-11	Mar-11	
	Complete review and selection of Strategic Alliance applications	Jun-11	Jul-11	Discussed in this report
	Implement new Strategic Alliance research tasks	Sep-11	Sep-11	Discussed in this report

NOTEWORTHY ACCOMPLISHMENTS

Subtask 4.7 researchers have hydrostatically pressure-tested the apparatus that they designed and had built, meaning that it was pressurized internally with water to beyond the working range that it will see during experimentation. Subtasks 4.3, 4.5, 4.7, and 4.9 are involved in collaborative research through performing testing and analyses on the same three samples from the Skyline 16 oil shale core (GR-1, GR-2, and GR-3).

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 be completed in the next quarter now that the four unconventional fuel development scenarios in Subtask 6.1 have been finalized. Subtask 4.7 has experienced slight delays with third party fabrication but anticipates returning to schedule in the upcoming quarter. There were also delays in Subtask 4.9 when it was determined that the kerogen used for the data reported last quarter still had mineral matter; most of the data, except for the SAXS work, has now been retaken on clean GR-1 and GR-2 kerogen samples.

RECENT AND UPCOMING PRESENTATIONS/PUBLICATIONS

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.

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

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

R. Keiter and J. Ruple. One source- Evolution of the policies surrounding ground & surface water management in the West. Presented at the University of Idaho Law Review's annual symposium, April 15, 2011.

R. Keiter and J. Ruple. Clear law and murky facts: Utah's approach to conjunctive surface and groundwater management, Idaho Law Review, 2011.

J. Ruple. Wild lands and wilderness – Implications for Utah's unconventional fuels industry. Presented at the 2011 University of Utah Unconventional Fuels Conference, May 17, 2011.

S. H. Lau, C. L. Lin, and J. D. Miller. 3D characterization of porous and multiphase materials with high contrast and multiscale resolutions. Paper presented at 4th International Workshop on Process Tomography, Chengdu, China, September, 2011.

J. H. Bauman, R. Bhide, and M. D. Deo. An evaluation of porosity and permeability changes in oil shale due to thermal stresses. Paper presented at the 31st Oil Shale Symposium, Colorado School of Mines, October 17-19, 2011.

A. Orendt, J. C. Facelli, and R. Pugmire. Atomistic modeling of oil shale kerogens and asphaltenes. Paper presented at the 31st Oil Shale Symposium, Colorado School of Mines, October 17-19, 2011.

A. Orendt, R. Pugmire, J. C. Facelli, and L. Birgenheier. Structural characterization of segments of a Green River oil shale core and the kerogen isolated from these segments. Paper presented at the 31st Oil Shale Symposium, Colorado School of Mines, October 17-19, 2011.

A. Orendt, R. Pugmire, J. C. Facelli, and L. Birgenheier. Detailed analytical data from select segments of a Green River oil shale core. Poster presented at the 31st Oil Shale Symposium, Colorado School of Mines, October 17-19, 2011.

T. Q. Tran, J. D. McLennan, M. Deo, and R. Okerlund. Evaluation of transport properties of in-situ processed oil shale. Poster presented at the 31st Oil Shale Symposium, Colorado School of Mines, October 17-19, 2011.

M. Vanden Berg and L. Birgenheier. Not all rich zones are created equal: Geologic characterization results of Green River formation core descriptions from Utah's Uinta Basin, including the newly drilled Skyline 16 core. Paper presented at the 31st Oil Shale Symposium, Colorado School of Mines, October 17-19, 2011.

M. Vanden Berg and L. Birgenheier. Geologic characterization of Green River oil shale. Abstract submitted to the annual meeting of the American Association of Petroleum Geologists to be held in April 2012.

C.L. Lin, J.D. Miller, C.H. Hsieh, P. Tiwari & M.D. Deo. Pore scale analysis of oil shale pyrolysis by X-ray CT and LB simulation. Paper is being revised and will sent to a peer-reviewed journal.

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." Manuscript can now be completed with data obtained this quarter.

I. S. O. Pimienta, Badu, A. M. Orendt, J. C. Facelli, and R. J. Pugmire, "Ab initio calculation and molecular dynamics simulation of asphaltenes." Manuscript being prepared for submission to *Energy & Fuels*.

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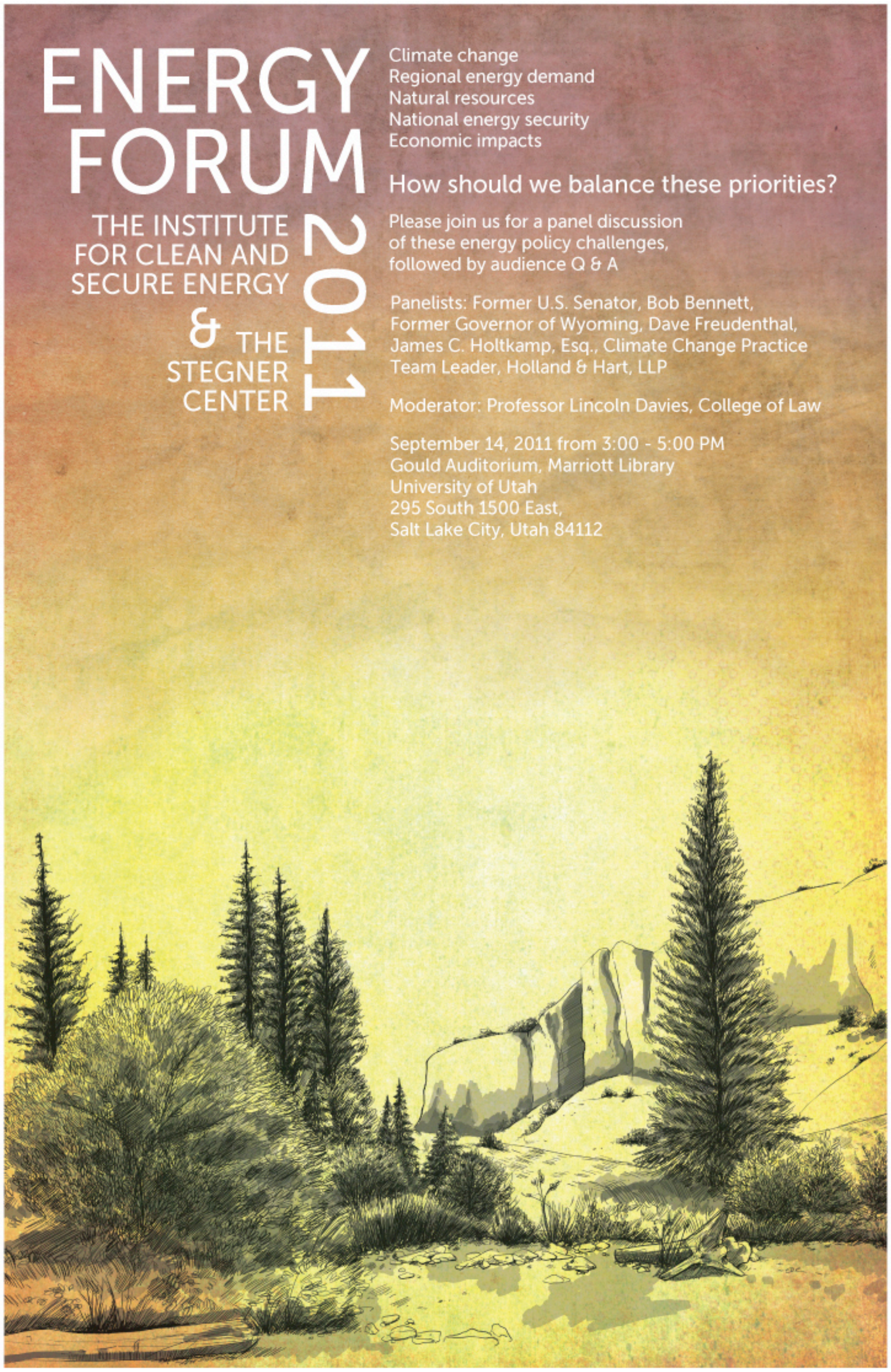
APPENDIX A. Promotional flyer for 2011 Energy Forum that was cosponsored by ICSE.



Institute for CLEAN AND SECURE ENERGY THE UNIVERSITY OF UTAH

Wallace Stegner Center for Land, Resources and the Environment University of Utah S.J. Quinney College of Law

S.J. QUINNEY COLLEGE OF LAW THE UNIVERSITY OF UTAH

APPENDIX B. Preliminary draft of the upcoming 2011 Advisory Board Meeting.

ADVISORY BOARD MEETING 2011

THE INSTITUTE FOR CLEAN AND SECURE ENERGY
THE UNIVERSITY OF UTAH

November 1, 2011
Warnock Engineering Building, Eccles Board Room

1:00 - 1:30 Welcome & Introductions, Professor David W. Pershing

1:30 - 2:30 ICSE Research & Financial Overview, Professor Philip J. Smith

2:30 - 2:50 Break

2:50 - 5:00 Research Project Presentations

6:30 - 9:00 Advisory Board Dinner

November 2, 2011
INSCC Conference room 345

8:30 - 9:00 Breakfast

9:00 - 10:00 The State of Climate Legislation, Professor Arnold W. Reitze, Jr.

10:00 - 10:20 Break

10:20 - 12:30 Advisory Board Discussion, Adjourn

Institute for CLEAN AND SECURE ENERGY
THE UNIVERSITY OF UTAH

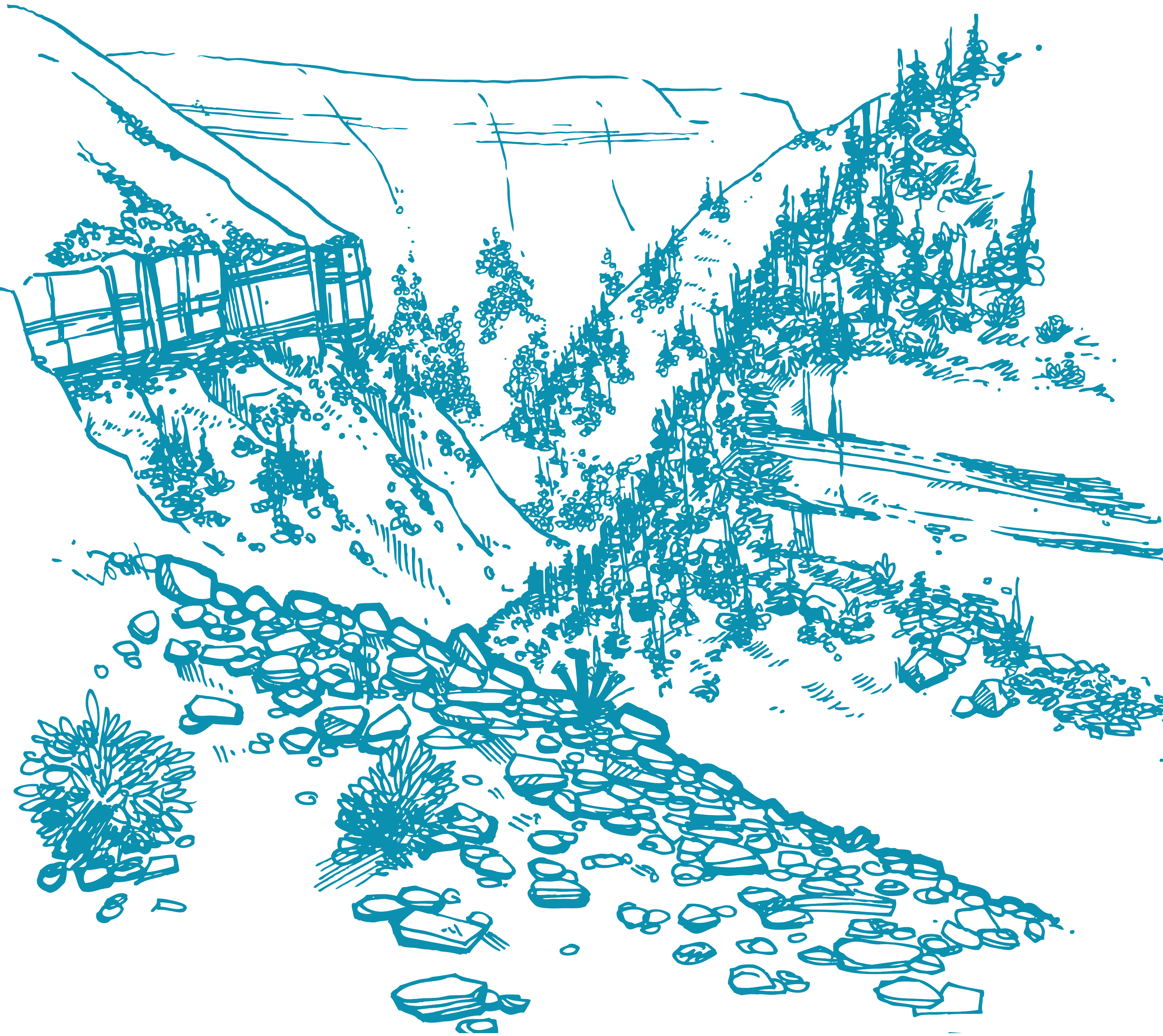
APPENDIX C. 2011 Advisory Board Update (see attached).

APPENDIX D. Well file data (see attached).

ADVISORY BOARD MEETING

2011 UPDATE

THE INSTITUTE FOR CLEAN AND SECURE ENERGY
THE UNIVERSITY OF UTAH



ICSE Advisory Board Update – August 2011

At the 2010 Advisory Board Meeting, the Advisory Board members in attendance* recommended strongly that ICSE should endeavor to forge closer ties to industry, and should actively seek to develop opportunities to participate in demonstration-scale research opportunities.** The consensus of the Board was that deeper ties to industry and the potential for demonstration-scale opportunities would (1) offer ICSE access to the experimental data needed to validate demonstration-scale ICSE simulations, (2) enable industry and policymakers to identify where simulation science could reliably and safely replace future experimental scale-up steps, and (3) thereby offer significant benefit to the public by effectuating more rapid deployment of emerging technologies.

This Update describes six collaborative projects between ICSE and various industry partners, ranging from nascent efforts to those already underway, which represent efforts to implement the Board's recommendation. The projects summaries included in this Update are:

For further information about these projects, please contact Kirsten Uchitel, kirsten.uchitel@law.utah.edu, or the principal contact(s) listed under each project.

** Board Members in Attendance at the 2010 ICSE Advisory Board Meeting: Ian Andrews, PacifiCorp Energy; Spencer P. Eccles, Utah Governor's Office of Economic Development; Jim Holtkamp, Holland & Hart; Hishashi "Sho" Kobayashi, Praxair, Inc.; John Marion, Alstom Power; Dianne Nielson, Utah State Energy Advisor; Laura Nelson, Red Leaf Resources, Inc.; David Pershing, University of Utah; Mark Raymond, Uintah County Commission; Kevin Shurtleff, Mountain West Energy, LLC; Joseph Strakey, Department of Energy, NETL; David Tabet, Utah Geological Survey; Andy Wolfsberg, Los Alamos National Laboratory Board Members Absent from the 2010 ICSE Advisory Board Meeting: Larry Crist, U.S. Fish &Wildlife Service; Robert Lestz, GasFrac Energy Services, Inc.; Larry Monroe, Southern Company; David Nimkin,National Parks Conservation Association.*

*** For purposes of the Board's discussion, demonstration-scale projects were defined as those projects that afforded ICSE researchers the potential to link their research to larger scale industrially driven demonstrations of technologies relevant to both industry and society. These are intended to be "life-scale" industrial projects towards which ICSE commits a portion of its federal funding dollars and its expertise, but which ICSE does not necessarily manage. Rather these projects are envisioned as group efforts designed to validate and advance a new technology or concept.*

The Oxy-Fuel Combustion CO_2 Capture Project

Principal Contact: Dr. Jeremy N. Thornock

A promising alternative to post-combustion CO_2 capture is using pure oxygen obtained from an air separation unit, combined with recycle gases, as the combustion oxidizer. The resulting combustion products contain mostly CO_2 and water, thus enabling drying and direct compression of the flue gas for sequestration or other CO_2 storage schemes. This approach to CO_2 capture eliminates flue gas separation processes, and provides an additional control to the combustion process. This approach is particularly attractive for retrofit applications because the boiler temperatures may be maintained at pre-retrofit conditions by using appropriate amounts of recycled flue gas combined with feed O_2 streams.

Technologies to increase energy efficiency will also result in reducing CO_2 footprints. The main obstacle for developing technologies with higher energy efficiency is the conflict between higher temperatures needed for higher efficiency and the resulting increase of thermal NO_x - formation (a major air pollutant). Industrial furnaces could reduce their energy consumption by 30 to 50% if they could use higher air preheat temperatures without increasing NO_x emissions. An emerging technology to accomplish this objective is flameless combustion.[1, 2, 3] Flameless combustion technology with oxy-firing provides potential for even further increases in energy efficiency while providing a path to capture the CO_2 produced in a variety of combustion processes.

Our objective is to demonstrate the coupling of science-based simulations with demonstration-scale experiments to provide quantifiable performance predictions of oxy-fuel and flameless retrofit power or thermal generation to speed the deployment in increased efficiency and CO_2 emissions reduction. Specifically, we aim to demonstrate the technology at a small furnace scale. The expected outcome is the creation of enabling technology to allow extrapolation from any existing air-fired operation to oxy-fuel and/or flameless operation. To achieve this with confidence requires robust validation and uncertainty quantification at a scale applicable to utility power production, a new generation of software tools for simulation, data mining, analysis, and access to peta-scale computing facilities, and integration of data from massively parallel simulations with data from a carefully designed set of validation experiments.

This program is focused on addressing crucial operational and design questions using high fidelity simulation for oxy-fuel and flameless systems of industrial scale furnaces. High-performance simulation tools are being used to assess the operational stability, primary CO_2 and O_2 feed optimization for CO_2 purity, recycle optimization, assessment of the effects of air ingress from imperfect furnace construction/design, and heat transfer efficiency to the radiant and convection sections of the furnace. The simulation objectives will be accompanied with quantified uncertainty through full V/UQ analysis. We are currently working with potential industrial partners to gather data as well as using those data in the open literature for pilot to full-scale geometries. These data are the observables required for the V/UQ activities.

Project deliverables include: advanced, high performance simulation software for the prediction of natural gas systems for retrofit applications; advanced radiation modeling using reverse Monte Carlo ray tracing techniques to improve computational efficiency and physical accuracy; advanced combustion modeling techniques; and V&V/UQ analysis for single burner, natural gas systems from lab to full scale.

[1] *C. Galletti, A. Parente, L. Tognotti, Combust. Flame 151 (2007) 649–664.*
[2] *J. A. Wünning, J. G. Wünning, Prog. Energ. Combust. 23 (1997) 81–94.*
[3] *A. K. Gupta, J. Eng. Gas Turbines Power 126 (2004) 9–19.*

Validation/Uncertainty Quantification for Large Eddy Simulations of the Heat Flux in the Tangentially Fired Oxy-Coal Alstom Boiler Simulation Facility

Principal Contacts: Dr. Philip J. Smith, Dr. Eric G. Eddings, Dr. Jost O.L. Wendt

The ultimate objective of this task is to produce predictive capability with quantified uncertainty bounds for the heat flux in commercial-scale, tangentially-fired, oxy-coal boilers. Data from the Alstom Boiler Simulation Facility (BSF) for tangentially fired, oxy-coal operation will be used for sub-scale validation. The results of the BSF simulations will be applied as appropriate to Alstom's 350 MWe oxy-coal demonstration design. This capstone project brings together Alstom's DOE project for measuring oxy-firing performance parameters in the BSF with this University of Utah (U of U) project for LES and V/UQ. The Utah work will include V/UQ support with measurements in the single-burner facility where advanced strategies for O_2 injection can be more easily controlled and data more easily obtained.

One of the outcomes of this task is to work with an industrial partner (Alstom) to transfer LES and V/UQ technologies to industrial application. This task forms the basis for bridging the Phase I through III university research on clean and secure energy from coal to industrial/commercial full-scale applications. This task will include the following subtasks:

(1) LES simulation and V/UQ for heat flux in Alstom oxy-coal-fired BSF

The objective of this subtask is to work directly with Alstom Power to apply the LES and V/UQ strategies developed under this research program to the Alstom BSF and 350 MWe oxy-coal demonstration design. The long-term objective of this research is a) to expand high-performance simulation tools to quantitatively predict the temperature and heat-heat flux in oxy-coal burners for retrofitting power boilers and industrial furnaces for CO_2 capture, and b) to perform verification, validation and uncertainty quantification of the numerical and modeling error associated with this intended use of the simulation tool. The work to be conducted under Phase 3 will take a large step towards this objective by bringing together the DOE funded research at both the U of U and at Alstom. In conjunction with Alstom Power, the Recipient shall focus on three activities: simulations of the BSF, application of knowledge to Alstom's 350 MWe oxy-coal demonstration design, and technology transfer.

(2) LES simulation and V/UQ for heat flux in subscale U of U oxy-coal-fired OFC

The objective of this subtask is to extend the simulation work being performed on applicable temperature and heat flux applications. Simulations of the U of U's 100 kW oxy-fuel combustor (OFC) appropriate to temperature and heat flux validation of the BSF will be performed by working with the experimental team under subtasks (3) and (4), described below. This simulation and validation work will be the underpinning for V/UQ of the larger scale BSF work of the LES simulation and V/UQ for heat flux in Alstom oxy-coal-fired BSF subtask.

(3) IR camera diagnostics & V/UQ for Temperature measurements in U of U OFC

The objective of this subtask is to develop and perform diagnostics for the OFC during its operation to be used for high-resolution model validation. Validation will be performed on both radiative flux and flame temperature based on infra-red (IR) imaging, as opposed to the temperature maps based on images obtained with emissions in the visible ranges performed with velocity measurements. To accomplish this subtask, ICSE researchers shall design, fabricate, and calibrate multiple wide-angle radiometers (2π steradians). The radiometers will first be calibrated with a black-body radiation source and then installed in the OFC reactor. In addition, researchers shall measure temperatures inside the OFC with a newly purchased high-speed infra-red (IR) camera. Researchers shall develop data-reduction methods to correlate pixel intensity to temperature. This camera will first be calibrated with a black-body radiation source and then mounted on the OFC reactor in cooperation with subtask (4).

Once these diagnostic capabilities are installed in the OFC, they will be used as part of thefor experimental verification and validation campaigns, as described in subtask (4). The radiometer and IR camera results from these tests will require data reduction and analysis, and researchers on all of the related subtasks will work together in order to integrate their measurement results with the simulation results and other experimental measurements.

(4) Heat flux profiles of UofU OFC using advanced strategies for O_2 injection

The objective of this subtask is to obtain validation data of heat flux and temperature profiles for axial flame simulations developed under subtask (2), and to make comparisons between oxy- and air- firing configurations. Data shall be obtained using diagnostic tools developed under subtask (3).

Retrofit Impacts of Oxy-coal Combustion of PRB Coal on Deposit Formation and Mercury Speciation

Principal Contacts: Dr. Jost O.L. Wendt, Dr. Geoff D. Silcox

Combustion of Powder River Basin, Wyoming (PRB) coal using oxygen rather than air (oxy-coal combustion) is potentially a viable technology for retrofitting existing coal-fired boilers for carbon capture and sequestration (CCS). The proposed research consists of two parts. The first part is concerned with determining the effects of oxy-coal combustion of PRB coals on boiler tube deposits, which can control boiler performance; the second part deals with the effects of oxy-coal combustion on mercury speciation, which plays a critical role in corrosion in CO_2 purification unit (CPU). Previous work at this laboratory has shown that, although effects of oxy-combustion on the size segregated elemental composition of the ash aerosol may be slight, the apparent effects on deposits may be significant, possibly because of differences in speciation. Previous mercury work at the University of Utah also suggests that oxy-firing can strongly enhance the oxidation of elemental mercury by chlorine.

The proposed research builds on these results and explores and quantifies how retrofit oxy-coal combustion configurations affect (1) the chemical and physical properties of deposits from PRB coals on specially designed deposit probes inserted in a 100kW oxy-coal combustion test rig and (2) the speciation of Hg in a laboratory quartz reactor and also in the coal fired test rig mentioned above. Two aspects of oxy-coal retrofit will be examined. First, effects of changes in recycled flue gas composition (with and without sulfur removal, with and without fine ash particle removal) will be examined; second, effects of changes in the amount of recycled flue gas (manifested as increased O_2 inlet concentration) will be examined. The focus will be on PRB coals (usually with high fouling propensity and non-soluble HgO emissions). An experienced team drawn from academia and industry will interpret data in the light of mechanisms, and make extrapolations to field conditions.

Fast Pyrolysis for Hydrocarbon Fuel Production

Principal Contact: Dr. Eric G. Eddings

Biofuel production needs to be increased significantly to meet the Renewable Fuel Standards of 36 billion gallons of biofuels per year mandated for U.S. consumers by 2022. Lignocellulosic biomass has been identified as a prime source for meeting such a fuel requirement, and one method for processing this biomass is through fast pyrolysis to yield a pyrolysis bio-oil, a pyrolysis gas and a bio-char. Each of these three products has significant value as a fuel; however, each can also be considered for their potential as higher-value commodities. The bio-oil can be further processed by hydrotreating for use as a refinery co-feed, or even further processed via catalytic cracking to produce hydrocarbons suitable for use as green transportation fuels. The bio-char can be used for soil amendment in agricultural applications, as a sorbent for CO_2 sequestration, or as a co-combustion fuel for heat or power generation. The pyrolysis gas could be used as a chemical feedstock, or it can be utilized as a fuel to fire a pyrolysis unit, such as the unit described below.

Professor Eric G. Eddings of the University of Utah, his doctoral student, Ben Coates, and Chief Engineer Dr. Ralph Coates, comprise the technical team of a start-up company called Amaron Energy, and they have developed a unique way to take renewable biomass (e.g., wood, algae, agricultural waste, food waste, turkey litter, etc.) and efficiently, and inexpensively, produce bio-derived oil in a carbon-neutral process. This bio-derived oil is somewhat similar to traditional petroleum crude oil, and can be upgraded to regular transportation fuels (diesel and gasoline). Traditionally, this bio-oil is produced with complex and expensive processes, such as fluidized bed reactors, to achieve what is called "fast pyrolysis." The Amaron Energy breakthrough is the development of an inexpensive rotary kiln process that is coupled with a precision control system to create a pyrolysis process that produces high quality bio-oil at a fraction of the cost of other fast-pyrolysis technologies.

Figure 1: Amaron Energy 1/2 ton/day prototype pyrolysis kiln.

Fast pyrolysis production of bio-oils has been extensively studied and a large fraction of biomass-based fast pyrolysis units are based on a fluidized bed design. In the Amaron Energy technology, the pyrolysis is accomplished with a uniquely designed, indirectly heated rotary kiln. Although pyrolysis in rotary kilns is customarily described in connection with slow pyrolysis, the Amaron kiln yields are very near those of fast pyrolysis fluid beds. Over the one and half years, Amaron Energy has designed and constructed a ½ ton per day prototype pyrolysis kiln, shown in Figure 1, and subsequently accumulated over 350 hours of testing with a variety of different materials including several types of wood, waste wood fines, sawdust, cow manure, turkey litter, brown grease, tires, waste plastic and lemna (a fast-growing energy micro-crop). A continuous 24-hour run was completed using pelletized wood, and there were no process upsets and just under 1 barrel of bio-oil was produced. While the residence time of the solids in the kiln can range up to 15 minutes, the residence time of the pyrolysis vapors is very short as demonstrated by oil yields exceeding 60%. Biochar is readily recovered as product in this process, in contrast to fluid-bed or many other pyrolysis technologies. The simplicity of the kiln design is well suited to the concept of

The University of Utah and Amaron Energy are partnering with Washakie Renewable Energy, a Utah-based company that specializes in the production of biodiesel and the distribution of various bio-derived oils. Washakie has production and distribution facilities in Utah, Texas and New Jersey, and has a strong interest in identifying new feedstocks sources. The current plan is to develop a 24-ton/day demonstration facility, and upon successful demonstration of the technology at that scale, the production of several commercial 200-ton/day facilities.

Mineralization: The Postcombustion Capture Program

Principal Contact: Dr. Sean Thomas Smith

While capturing near pure carbon dioxide (CO_2) for subsequent geological storage is one path for greenhouse gas (GHG) management, another technology option is extraction of the CO_2 from the flue gas of a conventional combustion system through mineralization to produce useable products. A technology that converts CO_2 from the burning of fossil fuel into carbon-negative building materials can enable the production of clean power, cement, fresh water and other products to promote sustainable growth. The process can capture other emissions, including sulfur dioxide, particulate matter, mercury, and other metals. For example, the Calera Carbonate Mineralization by Aqueous Precipitation (CMAP) process is a technology that converts CO_2 to carbonate (CO_3) and binds it to minerals such as calcium and magnesium. The output is a material composed of carbonate minerals that are stable across geological timeframes.

This above ground storage is a safe and environmentally sound alternative to geologic sequestration. Since the minerals are no longer in the form of carbon dioxide, long-term storage does not require monitoring, as does separated CO_2 geological storage. The byproducts of the process are carbonates used in the built environment. They can be transported from the production site to final consumers using existing infrastructure from the concrete industry.

CMAP, combined with a reverse osmosis unit, can produce fresh water from wastewater or brines. This process allows for a gain in energy efficiency in water treatment by demineralizing the water. This is particularly appealing in areas with abundant brines or seawater, but scarce fresh water. The water exiting the process can then be suitable for agricultural purposes or for conversion to potable water with far less treatment—and thus less energy expended—than the water entering the process. In areas with little water availability, even in a mineralized form, a limited supply of water can be recycled by remineralizing it with each introduction into the process.

Computational modeling and simulation holds potential for accelerating the deployment of this very new technology. Calera Corporation is working with the University of Utah to make bench, pilot and demonstration scale data available for verification, validation/uncertainty quantification of (V&V/UQ) simulation capability and process parameters. This program is organized in stages, each of which is discussed in turn.

CO_2 Absorption Column: Research shall focus on the simulation of a packed bed for CO_2 absorption. Attention is on performing V&V/UQ analysis with both ARCHES and Star CCM+. Development of simulation capabilities to accomplish this primary task will include building ARCHES infrastructure for handling complex packing geometry, multi-phase flow and chemical reactions. Research shall focus on creating simulations of a full geometry bed packing with CCM+ and an industrial-scale geometry packed-bed with modeled packing with ARCHES. Data shall be gathered from the open literature and from collaboration with mineralization industry. We are currently developing industrial partnerships for gathering data at bench, pilot and demonstration scales.

Mineralization Mixing Tank: Research shall focus on the simulation of an industrial sized stirred mixing tank for CO_2 mineralization with Ca and Mg cations. Attention is on performing V&V/UQ analysis with both ARCHES and Star CCM+. Development of simulation capabilities to accomplish this primary task will include building ARCHES & CCM+ infrastructure for handling large precipitation vessel designs and for including precipitation physics and chemistry (discussed under the Carbonate Precipitation brick). Research shall focus on simulations of an industrial-scale mixing tank with both ARCHES and CCM+. Data shall be gathered from the open literature and from collaboration with mineralization industries. We are currently developing industrial partnerships for gathering data at bench, pilot and demonstration scales.

Carbonate Precipitation: Research shall focus on the creation of a model for the mixing and reaction of carbonate precipitation. Carbonate precipitation reactions will be modeled with population balances which will be solved with direct quadrature method of moments. Attention is on the creation of the model incorporating appropriate nucleation, growth and aggregation kernels and on performing V&V/UQ analysis. One-dimensional turbulence (ODT) will be incorporated to bridge timescale discrepancies between nucleation and growth, providing a model for the Mineralization Mixing Tank project. The validated model will be applicable to both ARCHES and Star CCM+. Data for validation shall be gathered from the open literature.

Process Life-Cycle Analysis: Researchers shall develop an overall material and energy balance model for the mineralization process to help assess its feasibility. This will include minimum work calculations for reversible processes. Because the process produces several product streams: building materials, HCI, and fresh water, it will also be considered from a life-cycle perspective that includes life-cycle energy, raw material, processing, and disposal requirements for the three products. This task will also consider GHG emissions, and any critical inputs or outputs identified during the analysis. It will be based on general thermodynamic principles and publicly available process and life-cycle data. The effort shall focus on defining the parameter space (process, economic, and geographic) to ensure a viable process, even if it can be shown that this space is unobtainable. The space and its boundaries will be identified with attention to the possibility of using waste streams from other industrial processes, such as cement kiln dust, as sources of calcium ions and hydroxide ions for CO_2 absorption and mineralization.

Measuring & Controlling Combustion Efficiency of Industrial & Field Flares: Integrating Measurements and Simulations (University of Utah Proprietary/ new technology development)

Principal Contact: Dr. Philip J. Smith

Flaring waste streams of combustable material is an important control practice for destroying unwanted hydrocarbons and other combustable material. All studies performed to date have reached the conclusion that the proper operation of such flares produces near complete conversion of the hydrocarbons to combustion products. Thus, the focus of the US Environmental Protection Agency (EPA) in regulating flares has been to define proper operational procedures, assuming that if operated properly, the combustion efficiency would be near 100%. This proper operation has been defined in EPA's rule "General Control Device Requirements." [i, ii] However, defining proper operating procedures to ensure high combustion efficiency for the wide range of conditions that exist for actual flare operations is surely not only difficult (maybe impossible) but unwise.[iii] Since the regulatory goal is to achieve the highest possible combustion efficiency, it would seem wise to encourage creative technical solutions by promoting changes in both design and operations to achieve ever increasing combustion efficiency under an ever widening range of operating conditions.

Flare research over the past decade has increasingly illustrated that there is likely no one simple operational parameter (or even a few parameters) that will characterize the combustion behavior of flare flames.[iv] Simple correlations are unobtainable because of the complexity of the nonlinear mixing, reaction, and heat transfer present in operating flare flames. This complexity motivates the need to accurately measure combustion efficiency from operating flares so that the effect of different designs and operations can be quantified. However, this same complexity, makes such measurements difficult. To date there is no technology that has been been validated at providing quantitative combustion efficiency measurements from operating, open-air, flare flames.

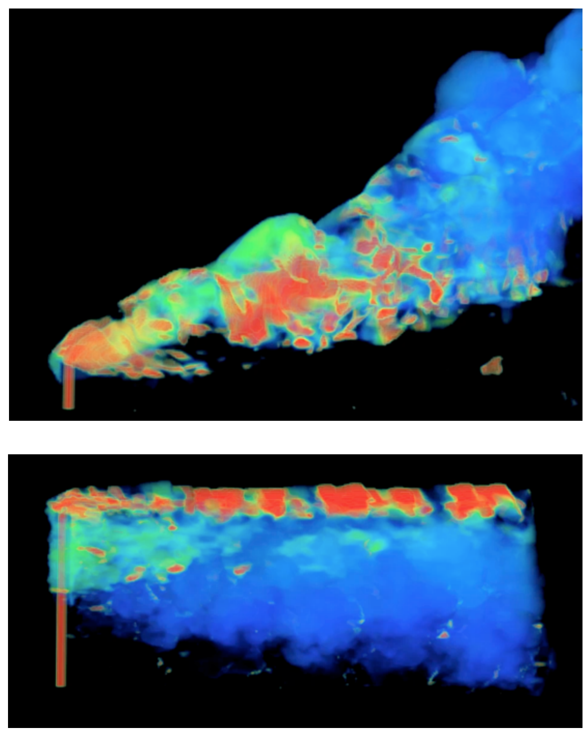


Figure 1: Heterogeneity in flare combustion efficiency as shown in these volume rendered images of a large eddy simulation (LES) of a field flare operating under two different crosswind conditions. Hot colors (red) represent high combustion inefficiency.

As illustrated in Figure 1, combustion simulations provide the opportunity to dynamically compute local heterogeneity to obtain quantitative combustion efficiency. However, the accuracy of these predictive simulations is directly affected by the uncertainty in the operating conditions of the flare. This uncertainty can only be quantified and reduced by coupling modern measurement and monitoring technologies with advanced computational simulation tools to root the prediction in actual measurements and operating conditions. To accomplish this task the simulation must be used to solve the verse problem instead of the forward problem. For example, heat flux is routinely measured from operating flares. One would like to use the HPC simulations to answer the question: if this is the measured heat flux from this flare what is the combustion efficiency? Using a predictive simulation tool to solve this inverse problem has historically been a difficult task. This dynamic coupled analysis approach to learning about a systems and moving it forward has been called a dynamic data driven application system (DDDAS).[v] It draws on the ability to incorporate additional measurement data into a simulation application and/or use simulation data to steer the application dynamically. The National Science Foundation has argued that DDDAS has the potential to transform the way science and engineering are done, and induce a major impact in the way many functions in our society are conducted (i.e. weather forecasting, oil exploration, etc).[vi] We are developing a DDDAS to 'measure' combustion efficiency from flares and use these measurements to dynamically adjust operating conditions to continuous operation at maximum combustion efficiency. This system requires the integration of: (1) modern high performance computer (HPC) simulations, (2) new formal uncertainty quantification methodologies, and (3) measurements of other measurable variables and operating conditions. Once integrated, this system will provide first, a continuous, real-time combustion efficiency 'measurement', and second, a control method to steer flare operation to continuously maximize combustion efficiency under ever changing operating constraints.

[i] *51 Federal Register (FR) 2701, Jan. 21, 1986, as amended at 63 FR 24444, May 4, 1998; 65 FR 61752, Oct. 17, 2000; 73 FR 78209, Dec. 22, 2008.*
[ii] *made available online by the National Archives and Records Administration at http://ecfr.gpoaccess.gov/.*
[iii] *For a further discussion of current EPA regulations see http://home.earthlink.net/~jim.seebold/id20.html.*
[iv] *The American Flame Research Committee (AFRC) of the International Flame Foundation (IFRF) has carried on a focused series of flare research forums. The papers from these forums are available online at http://www.afrc.net/index.jsp?page=1;&l2nid=6.*
[v] *Darema, "Dynamic Data Driven Applications Systems: A New Paradigm for Application Simulations and Measurements." International Conference on Computational Science.: pp. 662–669 (2004).*
[vi] *The term DDDAS was formalized by Frederica Darema around the time of a National Science Foundation (NSF) workshop in March 2000.*

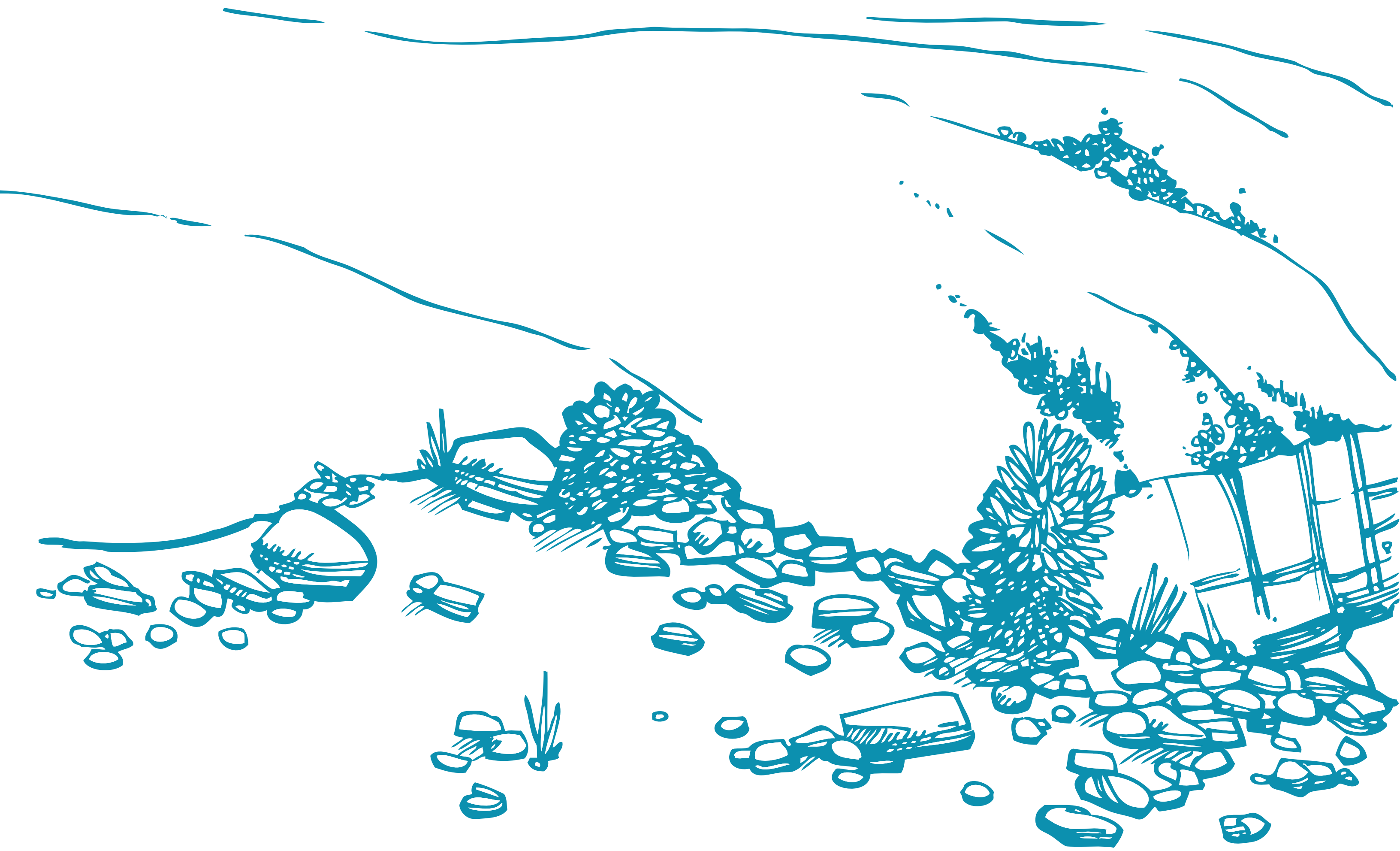


Table 1: Count of sampled wells with both drilling and completion cost, by year drilling commenced.

Year	2003	2004	2005	2006	2007	2008	2009	2010
Well Count	1	7	2	6	14	7	3	3

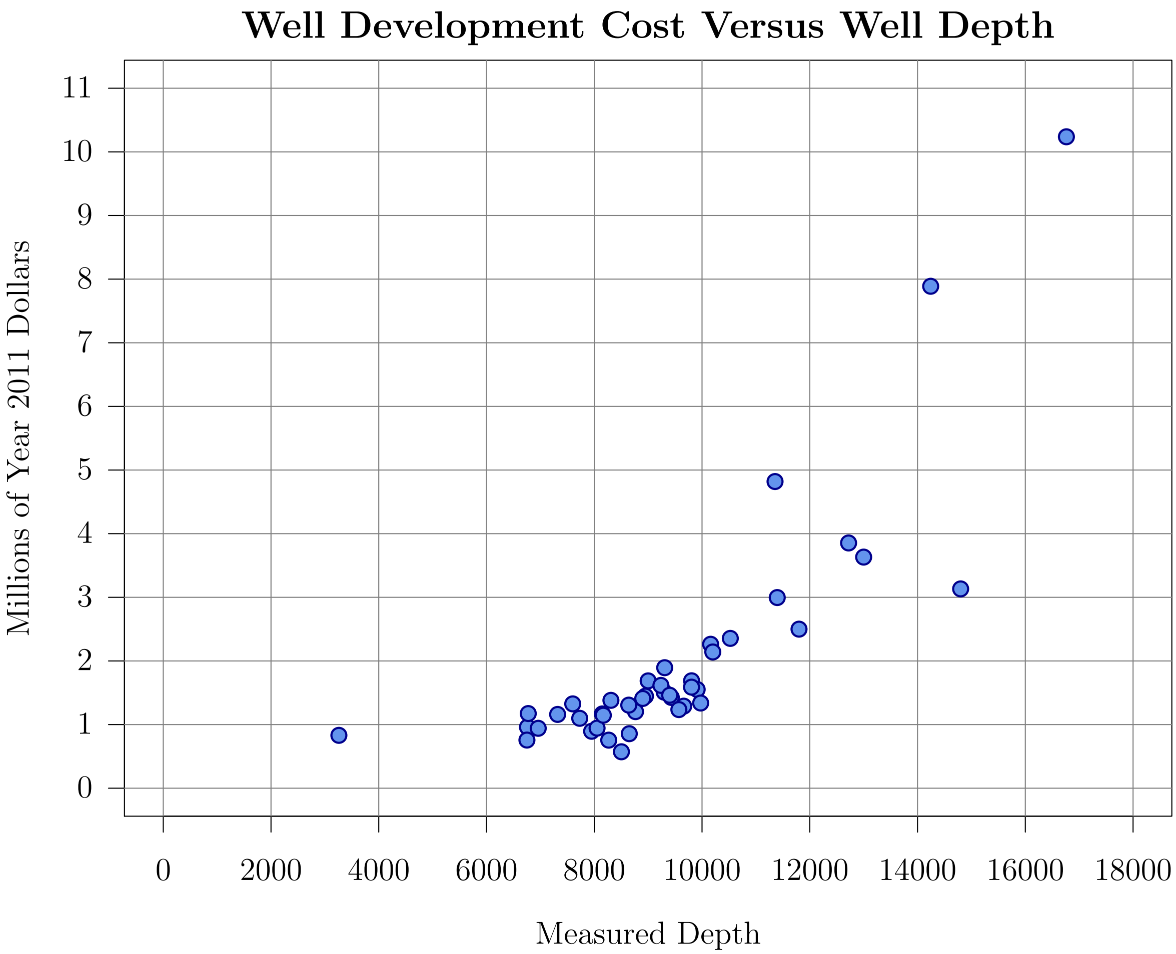


Figure 1: Note: Includes all and only wells with complete costs. Development costs are the sum of drilling and completion costs.

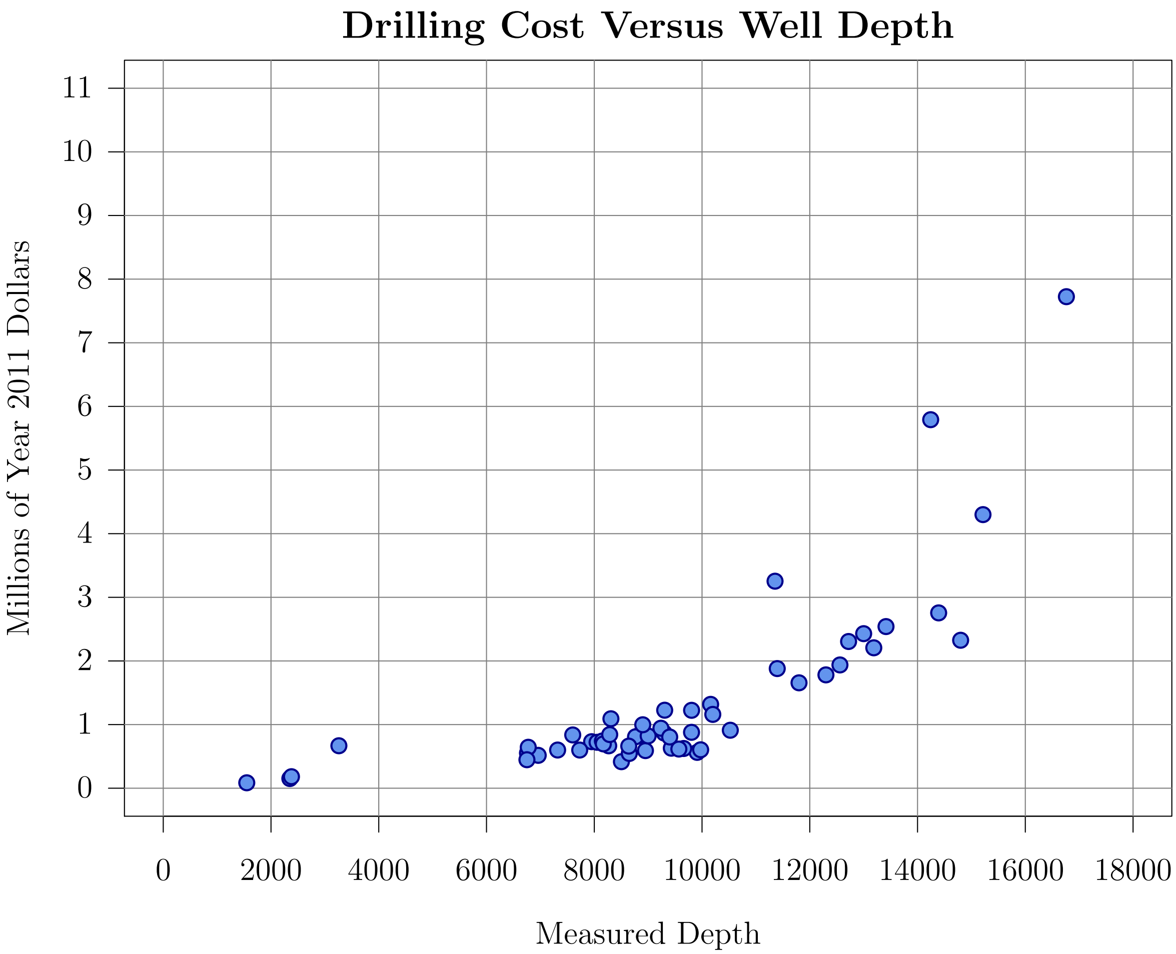


Figure 2: Note: Includes wells with complete costs and wells with only drilling costs.

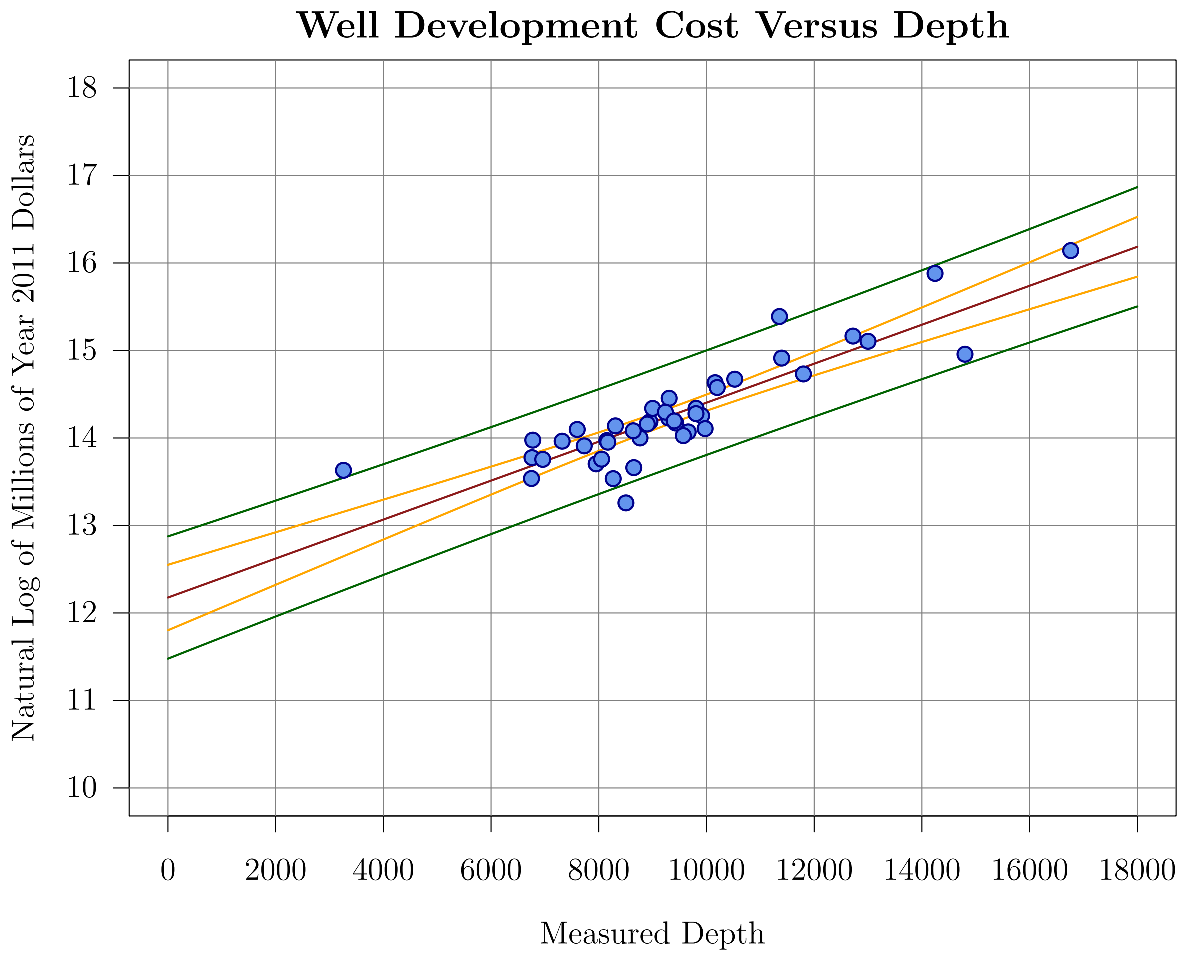


Figure 3: Model: $\log(\text{development}) = \alpha + \beta \cdot \text{depth} + \varepsilon$. Red line is the estimated expected response for a given depth. Orange lines are the upper and lower bounds of the confidence interval for the expected response, green lines are the upper and lower bounds of the confidence intervals for an individual response.

$$\log(\widehat{\text{development}}) = \widehat{\alpha} + \widehat{\beta} \cdot \text{depth}$$

Parameter estimates: $\widehat{\alpha} = 12.176$ and $\widehat{\beta} = 0.00022$.
Fit: $R^2 = 0.76912$.

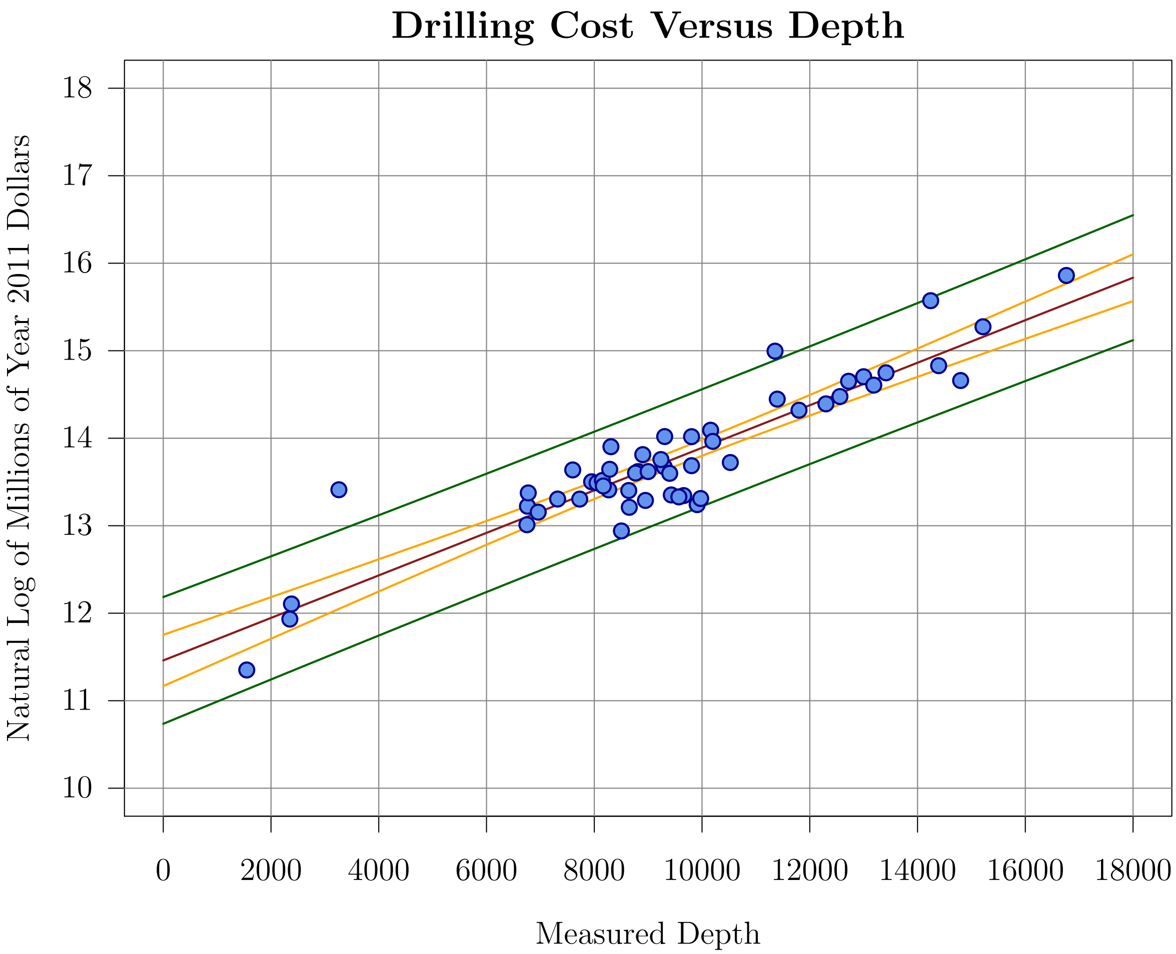


Figure 4: Model: $\log(\text{drilling}) = \alpha + \beta \cdot \text{depth} + \varepsilon$. Red line is the estimated expected response for a given depth. Orange lines are the upper and lower bounds of the confidence interval for the expected response, green lines are the upper and lower bounds of the confidence intervals for an individual response.

$$\widehat{\log(\text{drilling})} = \widehat{\alpha} + \widehat{\beta} \cdot \text{depth}$$

Parameter estimates: $\widehat{\alpha} = 11.46$ and $\widehat{\beta} = 0.00024$.
Fit: $R^2 = 0.84033$.

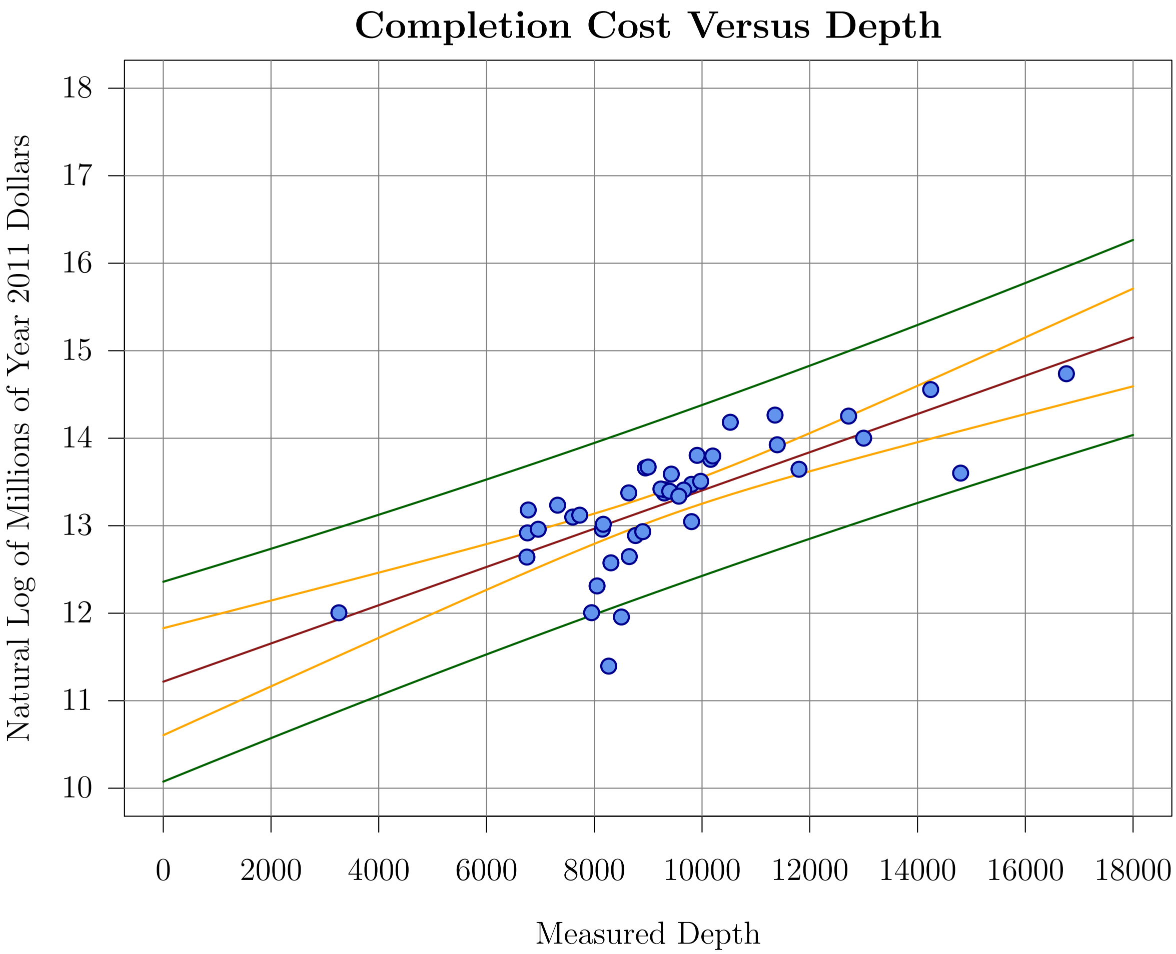


Figure 5: Model: $\log(\text{completion}) = \alpha + \beta \cdot \text{depth} + \varepsilon$. Red line is the estimated expected response for a given depth. Orange lines are the upper and lower bounds of the confidence interval for the expected response, green lines are the upper and lower bounds of the confidence intervals for an individual response.

$$\log(\widehat{\text{completion}}) = \widehat{\alpha} + \widehat{\beta} \cdot \text{depth}$$

Parameter estimates: $\widehat{\alpha} = 11.217$ and $\widehat{\beta} = 0.00022$.
Fit: $R^2 = 0.54565$.

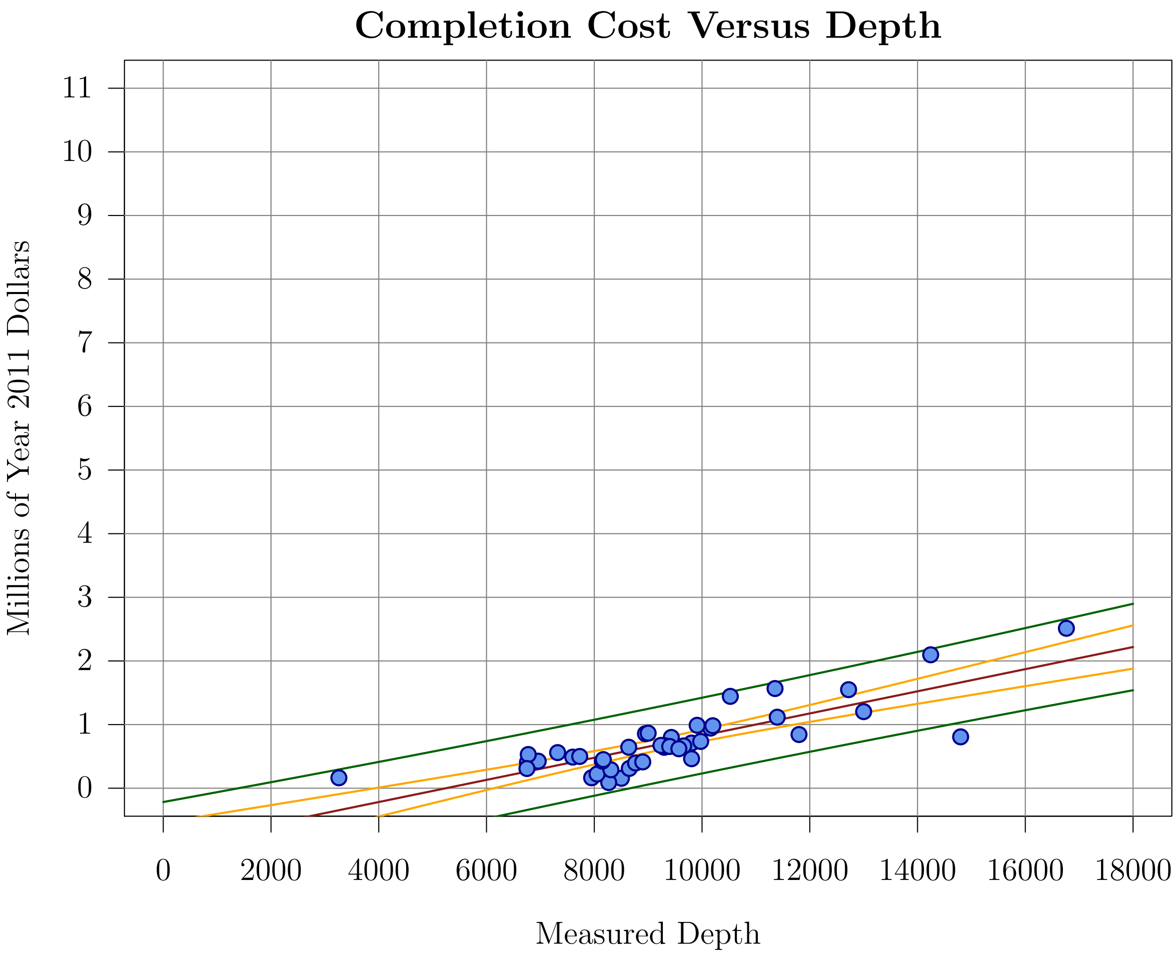


Figure 6: Model: completion $= \alpha + \beta \cdot \text{depth} + \varepsilon$. Red line is the estimated expected response for a given depth. Orange lines are the upper and lower bounds of the confidence interval for the expected response, green lines are the upper and lower bounds of the confidence intervals for an individual response.

$$\widehat{\text{completion}} = \widehat{\alpha} + \widehat{\beta} \cdot \text{depth}$$

Parameter estimates: $\widehat{\alpha} = -913176.6$ and $\widehat{\beta} = 173.995$.
Fit: $R^2 = 0.67203$.

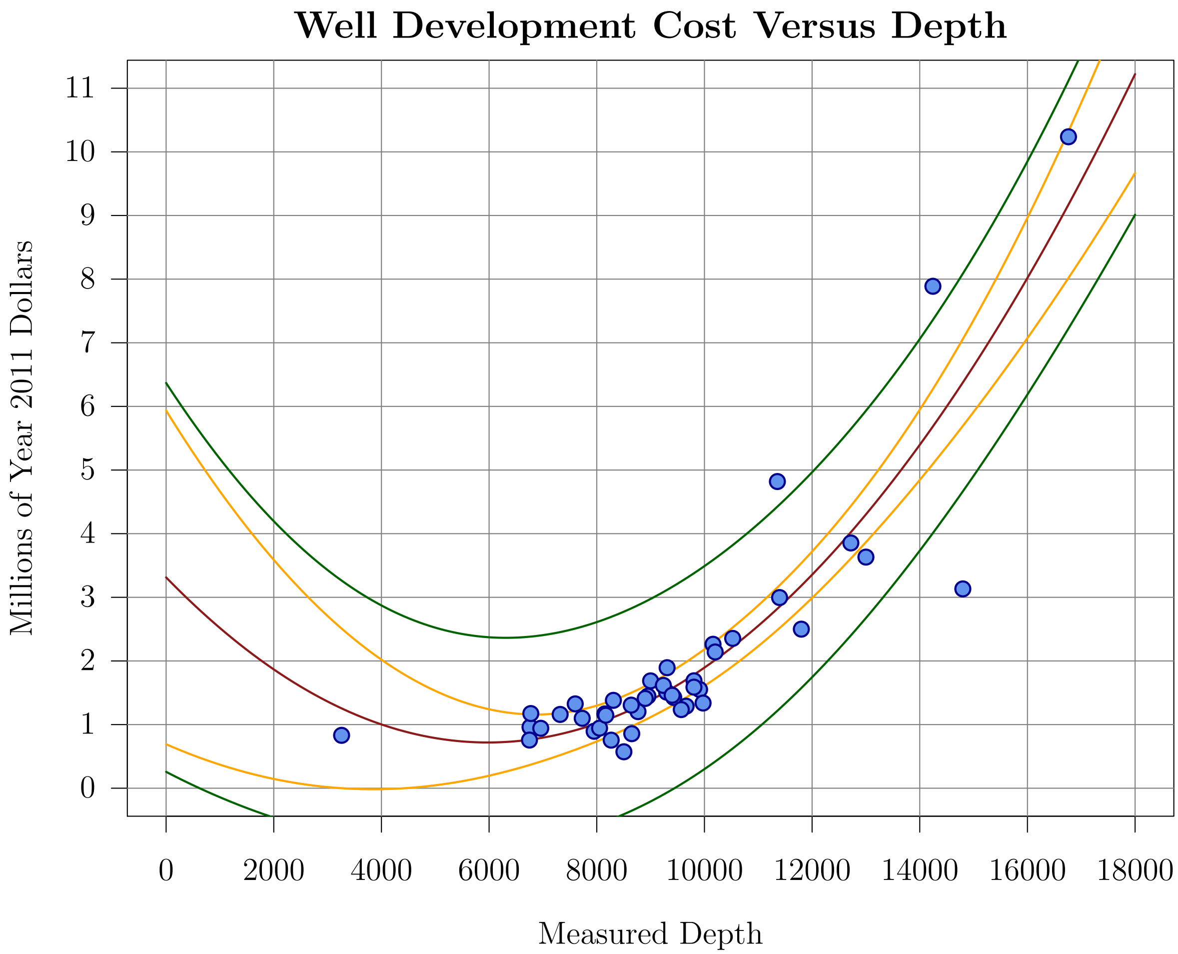


Figure 7: Model: development $= \alpha + \beta_1 \cdot \text{depth} + \beta_2 \cdot \text{depth}^2 + \varepsilon$. Red line is the estimated expected response for a given depth. Orange lines are the upper and lower bounds of the confidence interval for the expected response, green lines are the upper and lower bounds of the confidence intervals for an individual response.

$$\widehat{\text{development}} = \widehat{\alpha} + \widehat{\beta}_1 \cdot \text{depth} + \widehat{\beta}_2 \cdot \text{depth}^2$$

Parameter estimates: $\widehat{\alpha} = 3313146.6$, $\widehat{\beta}_1 = -868.264$, $\widehat{\beta}_2 = 0.07265$.
Fit: $R^2 = 0.82905$.

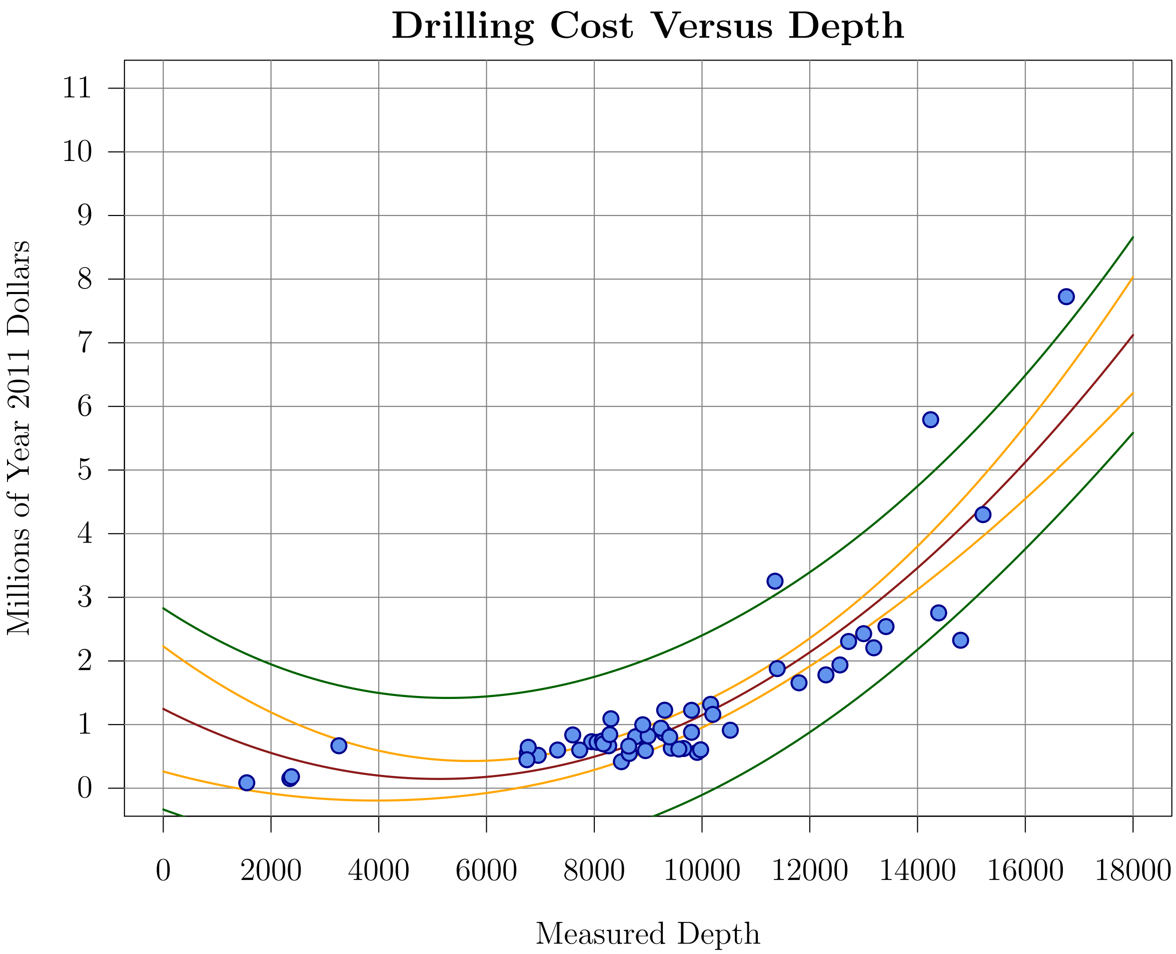


Figure 8: Model: drilling $= \alpha + \beta_1 \cdot \text{depth} + \beta_2 \cdot \text{depth}^2 + \varepsilon$. Red line is the estimated expected response for a given depth. Orange lines are the upper and lower bounds of the confidence interval for the expected response, green lines are the upper and lower bounds of the confidence intervals for an individual response.

$$\widehat{\text{drilling}} = \widehat{\alpha} + \widehat{\beta}_1 \cdot \text{depth} + \widehat{\beta}_2 \cdot \text{depth}^2$$

Parameter estimates: $\widehat{\alpha} = 1246980.9$, $\widehat{\beta}_1 = -430.313$, $\widehat{\beta}_2 = 0.04204$.
Fit: $R^2 = 0.80504$.

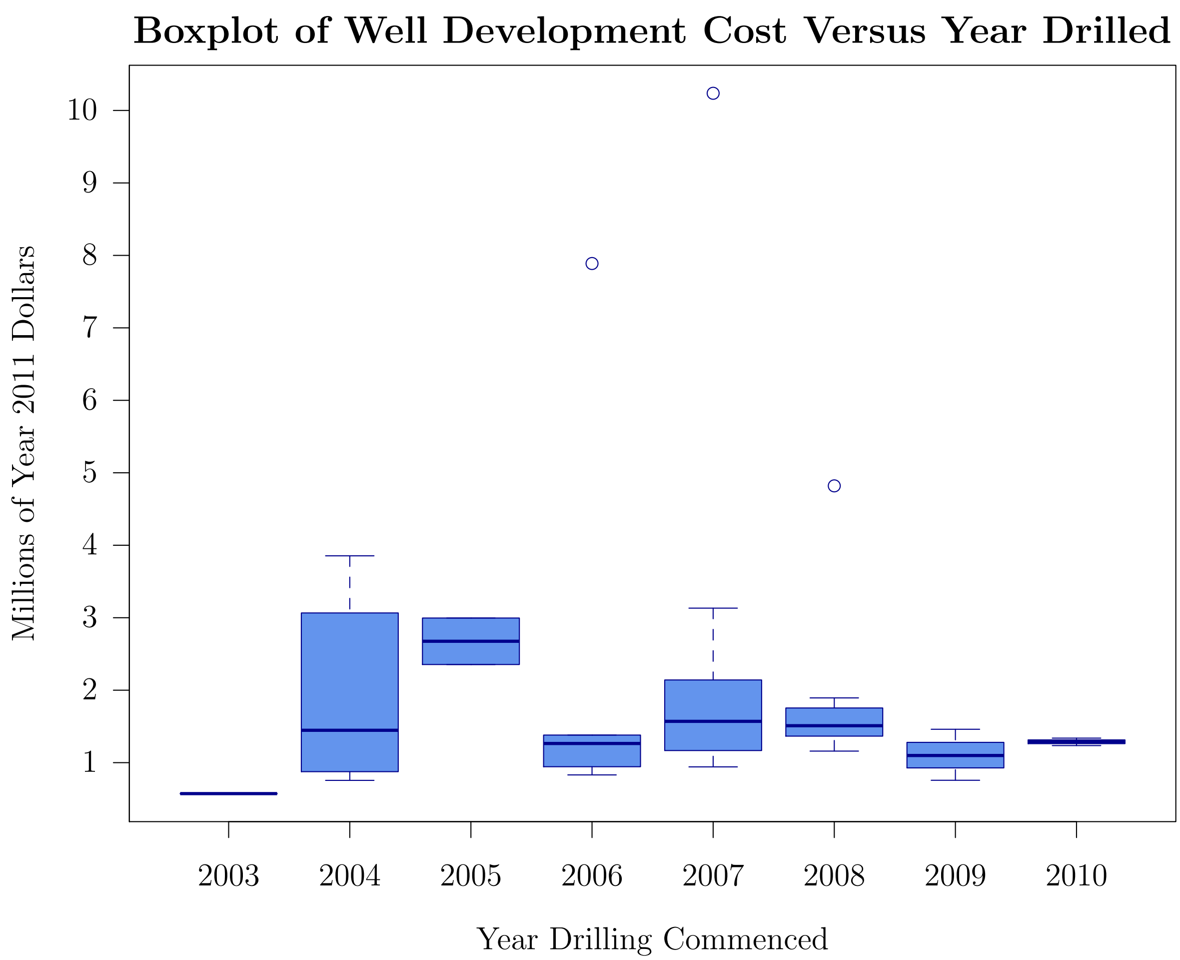


Figure 9: Note: The top of the box represents the 75th percentile, bottom of box represents 25th percentile, line inside box represents 50th percentile (median), ends of the "arms" represent endpoints of the range of data.

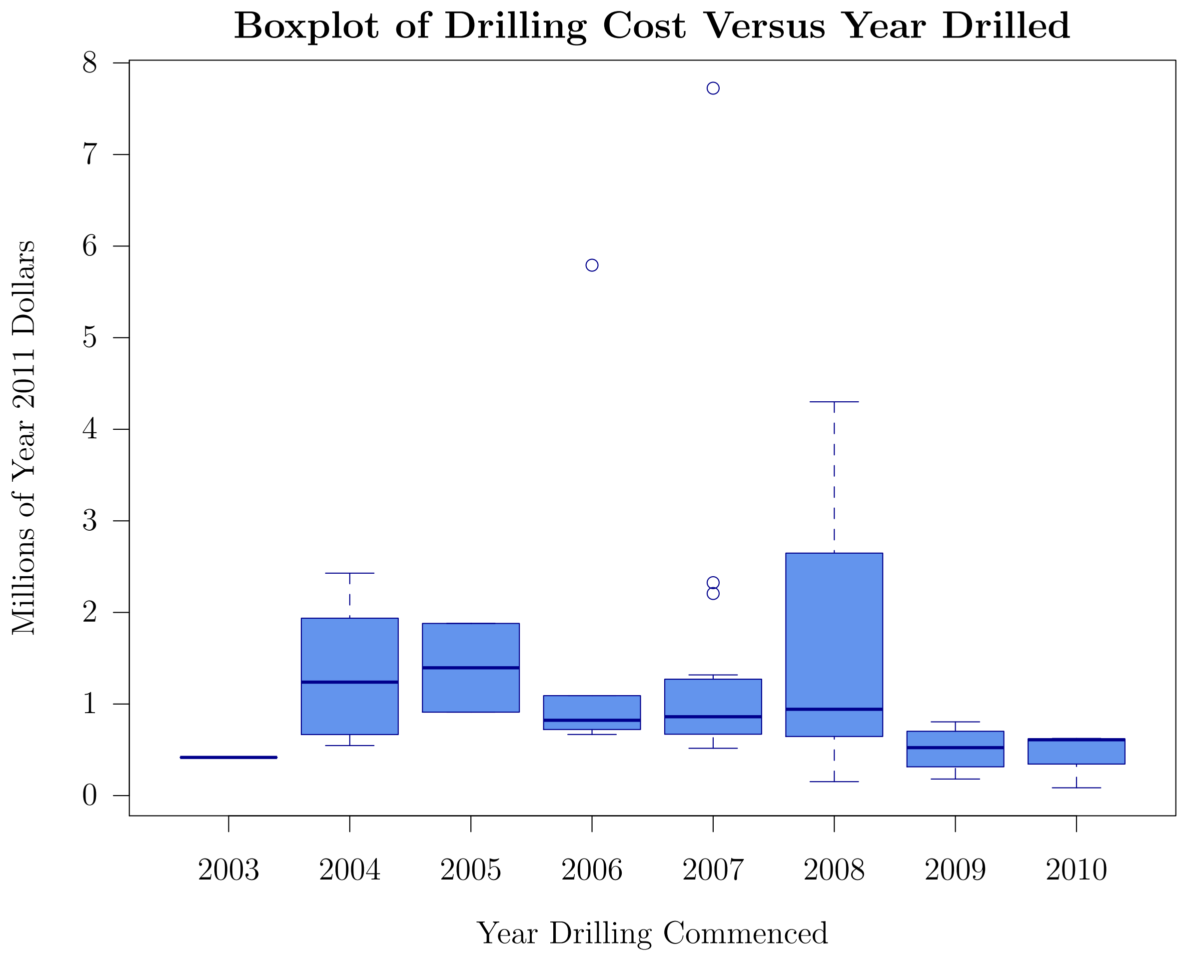


Figure 10: Note: The top of the box represents the 75th percentile, bottom of box represents 25th percentile, line inside box represents 50th percentile (median), ends of the "arms" represent endpoints of the range of data.

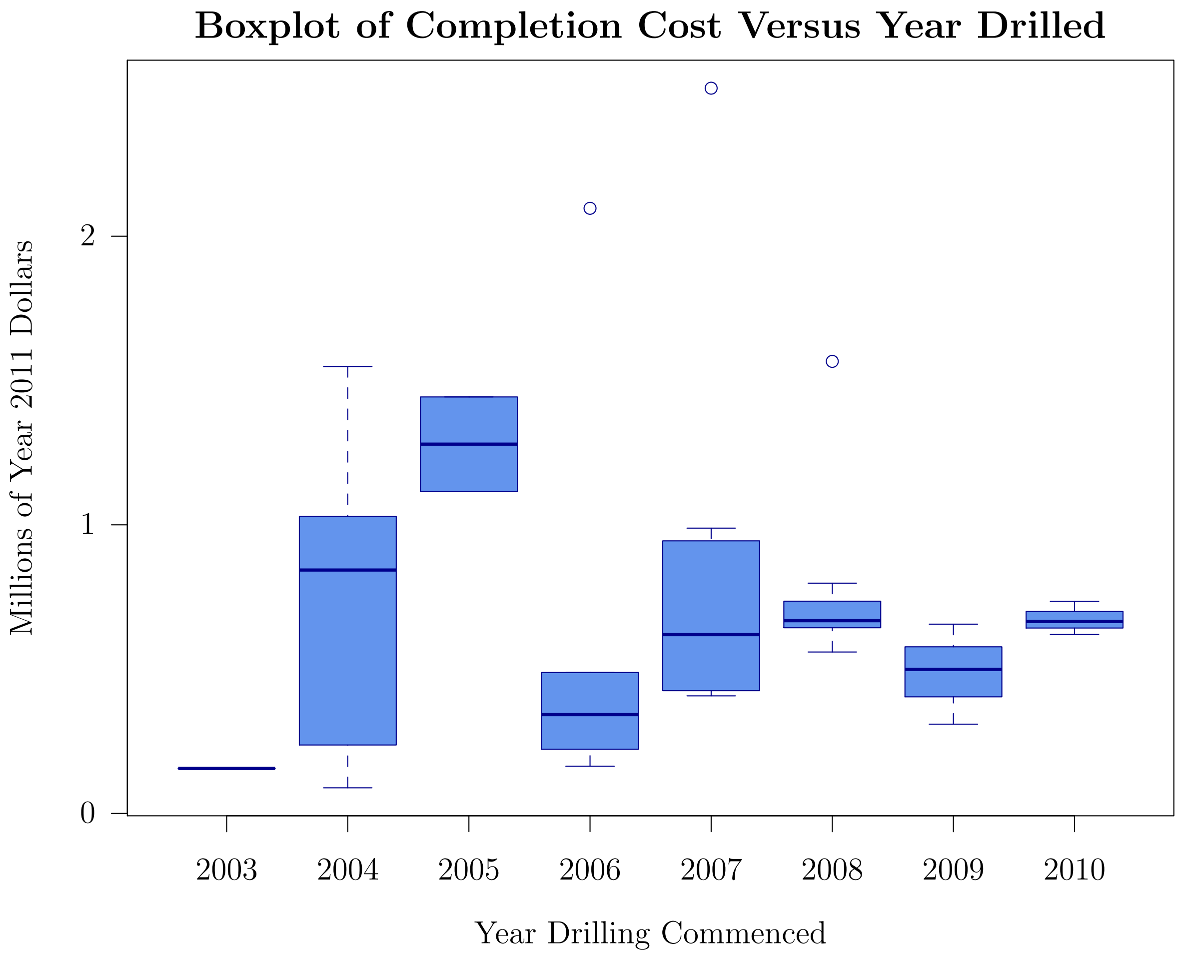


Figure 11: Note: The top of the box represents the 75th percentile, bottom of box represents 25th percentile, line inside box represents 50th percentile (median), ends of the "arms" represent endpoints of the range of data.

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