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 2014)

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

November 10, 2014

Office of Fossil Energy

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

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EXECUTIVE SUMMARY

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

Outreach efforts in Task 2 have continued to focus on disseminating results from the various subtasks and on fielding interview requests. Two papers from this program have been submitted for presentation at the 34th Oil Shale Symposium in Golden, CO, in October 2014.

Task 3 focuses on utilization of oil shale and oil sands resources with CO_2 management. The Subtask 3.3 and 3.4 teams improved their basin-scale conventional & unconventional fuel development model by performing a water balance for conventional oil and gas development, improving the conventional oil and gas drilling schedule model, and revising overall model into a centralized framework.

Task 4 projects are related to liquid fuel production by in-situ thermal processing of oil shale. The Subtask 4.3 project, reservoir simulation of reactive transport processes, was completed in this quarter; a topical report will be submitted in November 2014. Subtask 4.1 researchers incorporated a realistically-sized computational domain representing ex-situ retorting of a rubblized oil shale bed. However, excessively large computational efforts would be required to simulate oil shale retorting on a realistic time scale, so researchers will continue to improve our solution strategy. The Subtask 4.3 team continued work on a mechanistic model of oil shale kerogen pyrolysis based on the Chemical Percolation Devolatilization model. The elemental analysis of the chars showed that the carbon content does not change significantly at increased temperatures. A carbon balance and an aromatic carbon balance seem to suggest that the char should not be as aromatic as measured, unless significant ring addition reactions occur.

Task 5 and 6 projects relate to environmental, legal, economic, and policy analysis. A final topical report on policy and economic issues associated with using simulation to assess environmental impacts (Subtask 5.3) was submitted in early November 2014. All Task 5 and 6 projects are now complete.

Task 7 researchers are completing research on processes at a more commercially-relevant scale. The Subtask 7.3 team extended their in-situ simulation domain and ran three test cases to capture two years of heating in horizontal heater wells. They then compared the energy requirements of heating with the energy out in the form of oil produced. At the end of two years, the energy out to energy in ratio was not favorable for any of the three cases. They will continue to run simulations to capture longer retorting periods.

PROGRESS, RESULTS, AND DISCUSSION

Task 1.0 - Project Management and Planning

There were no schedule/cost variances or other situations requiring updating/amending of the Project Management Plan (PMP) in this quarter.

Task 2.0 -Technology Transfer and Outreach

Technology transfer and outreach efforts are focused on communicating project results through publication of papers and reports, through visits and interviews, and through updates of the program website. In this quarter, researchers in two subtasks had papers that were accepted for presentation at the 34th Oil Shale Symposium, held in Golden, CO, in October 2014 (see **Recent and Upcoming Presentations/Publications**).

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

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

In this quarter, the team focused on refining the information about emission factors associated with natural gas production and processing. This information will be used as part of the oil and gas production module to estimate greenhouse gas (GHG) emissions associated with oil and gas drilling operations in the Uinta Basin. The team is also attempting to identify the most appropriate emission factors for the Uinta Basin as well as to estimate the effect of the Environmental Protection Agency's (EPA) New Source Performance Standards (NSPS) on emissions.

For the same process, some emission factors vary by orders of magnitude. These differences are most likely due to different conditions at the study sites and different study methods. For example, formation properties and well productivity affect emissions. In addition, the emission factors come from three types of studies: industry surveys, emission measurements made on individual operations or pieces of equipment, and regional (top-down) measurements that use techniques such as species ratios to resolve oil and gas emissions from various sources. The survey-based studies tend to report lower emissions than the other two types. It is possible that the measurements performed at individual locations may not be representative of the industry as a whole because companies who volunteer for measurements may be the best actors and the properties of the sites may differ widely. The top-town measurements tend to report highly variable emission estimates, with some as high as 17% of natural gas emitted. Because many of the oil and gas producing regions also have natural gas seeps, it can be difficult to resolve natural gas activities from naturally-occurring sources.

During the site preparation through well completion phases of the process, well completion, in particular the flowback period, is the largest source of emissions and has a high degree of variability as seen in Figure 1. During production, fugitive emissions from a variety of sources, including liquid unloadings, pneumatic devices, compressor seals and tanks, are important; emissions from these sources also vary widely.

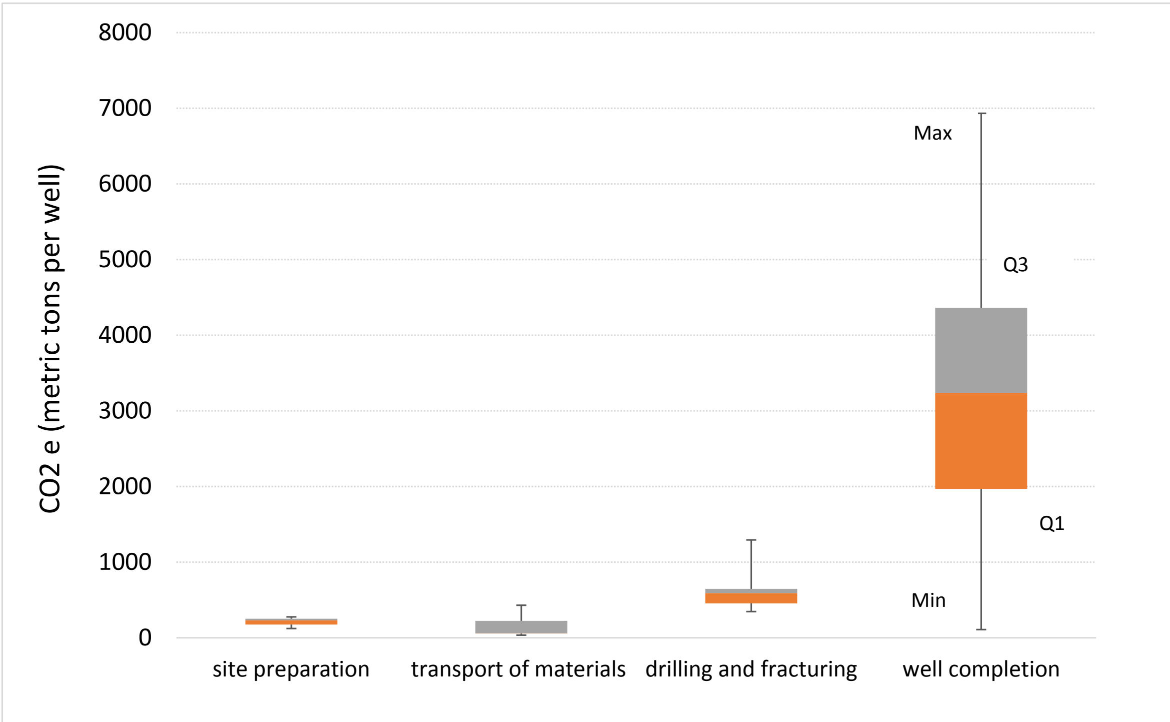

Figure 1. Median, 25th and 75th percentile, and minimum and maximum reported CO_2 equivalent (CO_{2e}) emissions per well.

Recommended emission factors

There are limited published emissions for tight-gas/tight sand formations in general and the Uinta and Piceance Basins in particular. However, the National Energy Technology Laboratory (NETL) estimates that emissions from tight gas and shale formations are similar (NETL, 2014). Karion et al. (2013) estimate that between 6.2–11.7% of natural gas produced is emitted in the Uinta Basin, while Petron et al. (2012) estimate losses of 1.7–7.7% from the Piceance Basin tight-gas formation. These estimates compare to an EPA nationwide average of 0.5% (EPA, 2013). Utah State University's (USU) Uinta Basin Winter Ozone & Air Quality Study (USU, 2012) reports that 0.013% of natural gas produced is emitted. The study also reports methane (CH_4) emissions from well completions and work overs that seem much lower (0.157 metric tons CO_{2e}/ spud) than those reported in other studies (483–6900 metric tons CO_{2e}/well). In addition, the USU study estimates fugitive pipeline emissions as 48.5 metric tons CO_{2e} / billion cubic feet of natural gas production. This value is also much lower than the values reported in other studies (665–1108 metric ton CO_{2e}/billion cubic feet of natural gas).

Table 1 shows the range of CO_{2e} and methane emissions for conventional and unconventional sources from natural gas extraction. In this report unconventional sources denotes to sources that require hydraulic fracturing technologies.

Table 1. CO_2 and CH_4 emission factor summary .

Activity	CO_{2e} conventional	CH_4 conventional	CO_{2e} unconventional	CH_4 unconventional	CO_{2e} EPA	CH_4 EPA	Units
well completion & workover	12-15	0.57-0.71	1841-2038	87.7-97.05			Metric tons/ billion cubic feet of natural gas production[1]
	12-36	0.57-1.71	38-3171	1.80-151	1701	81	Metric tons/ well[2]
			2971-6933	141.5-330.1	3171	151	Metric tons/ well[3]
Production	1.42-2.75	0.067-0.13	2.01-7.9	0.096-0.38			Expressed as % of total production
Processing	533-600	3.3-3.8	1994-2267	12.34-14			Metric tons/ billion cubic feet of natural gas production
Transmission	1108	52.76	1108	52.76			Metric tons/ billion cubic feet of natural gas production
Distribution	665	31.66	665	31.7			Metric tons/ billion cubic feet of natural gas production
Transport			34-431	1.62-20.52			Metric tons/ well

[1] Estimated as 10% of all gas vented.
[2] These values include both controlled and uncontrolled emissions.
[3] Entire volume of gas release during flowback.

Table 2 shows the average values for CO_{2e}, CH_4 and the estimates for non-methane volatile organic carbons (NMVOCs) for all basins and the best estimation for the Uinta Basin. Table 3 shows the emission factors recommended by the project team.

Table 2. Average CO_{2e}, CH_4 and NMVOC emission factors with available standard deviations.

	CO_{2e} average all basins	CO_{2e} average Uintah /tight gas /Rocky mountain [1]	CH_4 average all basins	CH_4 average Uintah /tight gas /Rocky mountain[1]	NMVOCs[2] average all basins	NMVOCs[2] average Uintah/tight gas/Rocky mountain[1]
Total % loss (% of methane over the lifecycle of a well)			1.76±1.15	**0.95±0.4**		
Total % loss (% of methane expressed as a percentage of total production)			4.9±3.5	**6.8±4.1**		
Site preparation (metric tons/ well)	208±78					
Drilling (metric tons/well)		1.05		0.05		0.0
Drilling and fracturing (metric tons /well)	737±369					
Transport of materials (metric tons /well)	160±169					
Well completion (metric tons/well completion)	2541±1579[3]	**1940.4±46[4]**	158.9	**92.4**	15.85	9.22
Processing (metric tons per billion cubic of natural gas produced)	1349±910		8.35[5]		0.84	
NG transport & distribution (metric tons per billion cubic of natural gas)	1773	48	84.4	2.3	8.42	0.23

[1] Includes estimates from tight gas, Uinta Basin and Rocky Mountains.
[2] NMVOCs emissions were calculated based on the natural gas composition for the Uinta Basin (mass basis) reported by Zhang et al. (2009) and Rice et al. (1992) (CH_4 86.4%, C_2H_6 8.56%, NMVOC 8.62% , VOCs 0.06 % and CO_2 1.75%). For this report, the definition of VOC is the result of subtracting methane, ethane (C_2H_6), nitrogen (N_2) and CO_2 from the total natural gas emitted.
[3] Only emission factors from unconventional sources were included. Value includes both controlled and uncontrolled emissions.
[4] Corresponds to the average of the emission factors reported by O'Sullivan et al. (2012), NETL (2014), API (2012), and Allen et al. (2013). NETL report accounts for the lower reservoir pressures of tight wells. NETL assumes that the emission factor for tight wells completion is about 40% of the emission factor for shale gas wells completion. Bold values signify recommended values for the Basin. This value includes both controlled and uncontrolled emissions.
[5] The contribution of methane to the CO_{2e} emissions from processing activities before NSPS implementation was estimated to be around 13% (based on NETL, 2014). This same percentage was applied to estimate the methane contribution from processing activities.

Table 3. Best estimates of emission factors for the Uinta Basin.

Activity	CO2e	CH4	NMVOCs	units
Site-preparation (excluding drill rig transportation) [1]	208±79	9.9	0.99	metric tons/well
Transportation of materials[2]				
Drilling	0.40	8.63E-06		metric tons/spud
Completions	0.21	4.36E-06		metric tons/spud
rework	3.05	7.17E-05		metric tons/spud
Production	1.36	3.29E-05		metric tons/well
Well drilling and fracturing[3]	737±369			metric tons/well
Well completion[4]	1940±46	9.24E+01	9.22	metric tons/well completion
Production[5]	99.80	4.75	0.47	metric tons/year well
Processing[6]	901±46	5.58	0.56	metric tons/billion cubic feet of total natural gas production
Transmission & distribution[7]		1.04 ± 0.85	0.1	percentage of methane produced over the lifecycle of a well

[1] Corresponds to the average of the emission factors by Jiang et al. (2011) and Santoro et al. (2011).
[2] From mobile sources based on an EPA study of transportation emissions associated with onshore oil and gas development in the Piceance Basin of Northwestern Colorado (EPA, 2011).
[3] Jiang et al. (2011).
[4] Corresponds to the average of the emission factors reported by O'Sullivan et al. (2012), NETL (2014), API (2012), and Allen et al. (2013). NETL report assumes that tight gas well completion emission factor is 40% of the emission factor for shale gas wells completion. This value includes both controlled and uncontrolled emissions.
[5] Value for Rocky Mountain region (Allen et al., 2013). This value includes both controlled and uncontrolled emissions.
[6] Corresponds to the average of the emission factors reported by Burnham (2011), Jiang et al. (2011), NETL (2014) and Canadian Association of Petroleum Producers (1999). This value includes both controlled and uncontrolled emissions. The contribution of methane to the CO_{2e} emissions from processing activities before NSPS implementation was estimated to be around 13% (based on NETL, 2014). This same percentage was applied to estimate the CH_4 contribution from processing activities.
[7] Corresponds to the average of emission factor values reported by Howarth et al. (2012) for several studies. These values include both controlled and uncontrolled emissions.

Table 4 presents the most relevant ranges for CO_2 and CH_4 emissions related to production and transport of oil. Limited studies related to the emissions of oil extraction activities were found in the literature.

Table 4. CO_2 and CH_4 emission factors for oil extraction activities.

Activity	$CO_{2}e$ emission factors	CH4 emission factors	VOC emission factor	Units
Production	1.69E-5 - 8.13E-5 [1]	8.05E-7- 3.87E-6[1]		metric tons/bbl
Transport	1.15 E-3 [2]	2.820E-07[2]	3.84E-07[2]	Metric tons/bbl transported

[1] Ranging from conventional to heavy oil.
[2] CO_2, CH_4, N_2O and VOC emissions for Heavy-Heavy Duty Truck from GREET (2014). CO_{2e} estimated for Global Warming Potential (GWP) of 1 for CO_2, 21 for CH_4 and 310 for N_2O. Average distance from the oil reservoirs to Daniel's Summit Lodge (Heber) is 121 miles. Crude oil is assumed to be carried out by trucks with an average capacity of 200 barrels (UBET, 2013).

Effect of new regulations

The EPA has recently finalized NSPS's for the oil and natural gas sector (EPA, 2012a). The EPA proposal for a NSPS (EPA, 2011b), the background technical support documents for the rule (EPA, 2012c) and the proposal (EPA, 2012b) provide a review of best practices for well completions and recompletions, pneumatic controllers, compressors, storage vessels and equipment leaks. After the NSPS implementation, the emission factors that can be used to estimate the emissions for new wells are presented in Table 5.

Table 5. Emission factors for CO_{2e}, CH_4 and NMVOCs after the NSPS implementations (NETL, 2014). Italic font indicates the percent increase in emissions after the NSPS implementation.

	CO_{2e} emissions (metric tons CO_{2e}/billion cubic feet)	% reduction or increase (metric tons CO_{2e}/billion cubic feet)	CH_4 emissions (metric tons CH_4/billion cubic feet)	NMVOCs (metric tons NMVOCs/billion cubic feet)
Construction	144.0	*2.0*		
Completion	14.1[1]	96.4	0.576	0.057
Production	720.8	65.8	18.17[2]	1.81[2]
Processing	3094.7	15.3	31.53[3]	3.11[3]
Transport	3182.6	*0.5*	101.95[4]	10.17[4]

[1] This completion emission factor was estimated as 40% of the emission factor for shale gas well completion as suggested in the NETL (2014) for tight wells.
[2] Based on the NETL (2014) data. CH_4 emitted due to water delivery and water treatment activities were not included.
[3] Based on the NETL (2014) data. Value assumes that emissions from other point sources and valve fugitives are mainly due to CH_4.
[4] Based on the NETL (2014) data. CH_4 emitted due pipeline construction was not included.

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

The project team encountered several bugs in the ARCHES simulation software during efforts this quarter to perform simulations of the IFRF oxy-fuel furnace using output from STAR-CCM+ as the inlet boundary condition. Researchers have been working closely with code developers to eliminate these bugs.

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

During this quarter, research in Subtasks 3.3 and 3.4 has focused on the following items:

- Developing a water balance for conventional oil and gas development
- Improving the conventional oil and gas drilling schedule model
- Revising the conventional oil and gas development model into a centralized framework

Progress on each of these items is detailed below.

Water Balance

Based on previous approaches to modeling water balances for oil and gas drilling (Goodwin et al., 2012) and discussions with experts in the water use practices in the Uinta Basin, the research team defined the water balance as depicted in Figure 2.

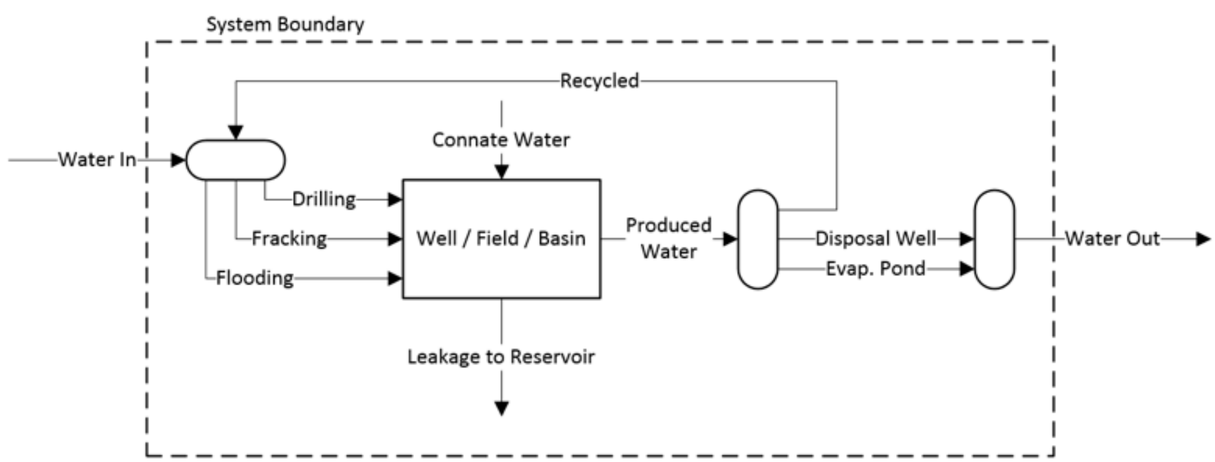

Figure 2. Water balance for conventional oil and gas water development.

Conventional oil and gas wells use water during drilling (for drilling muds and cement), completion (for hydraulic fracturing), and secondary recovery in oil wells (for water flooding). Water is produced from oil and gas wells during the flowback period following hydraulic fracturing and afterwards throughout the life of the well as part of production (whether from connate water in the reservoir or from water pushed through the reservoir as part of water flooding). Produced water is disposed of primarily through reinjection in disposal wells or evaporated in surface ponds. The difference between the reported amounts of water disposal and produced water is assumed to be recycled. The amount of water entering the system boundary can be quantified using the following set of equations:

(recycled) = (produced) - (disposal well + evaporated) (1)
(water in) = (drilling + fracking + flooding) - (recycled) (2)
(water intensity) = (water in) / (oil/gas produced) (3)

Researchers collected data on each of the terms listed in Equations (1)–(3) from a variety of sources. Utah's Division of Oil, Gas & Mining (DOGM) maintains public databases related to water: produced, disposed of through injection wells or evaporation ponds, and injected as part of water flooding projects (DOGM, 2014). DOGM also maintains records of well drilling activity reports for each well that either specifically states (for cement usage) or provides enough details to infer (for drilling mud) the amount of water used during drilling (DOGM, 2014). Finally, DOGM has required that all wells drilled since 2012 report their hydraulic fracturing usage to the website fracfocus.org (FracFocus, 2014). By combining information from all of these sources, the project team was able to get enough information to estimate the water usage for oil and gas wells in the Uinta Basin based on well depth and type using regression formulas fitted to each term in Equations (1)–(3). An regression example is shown for determining the amount of water produced as a linear function of the amount of oil produced is shown in Figure 3.

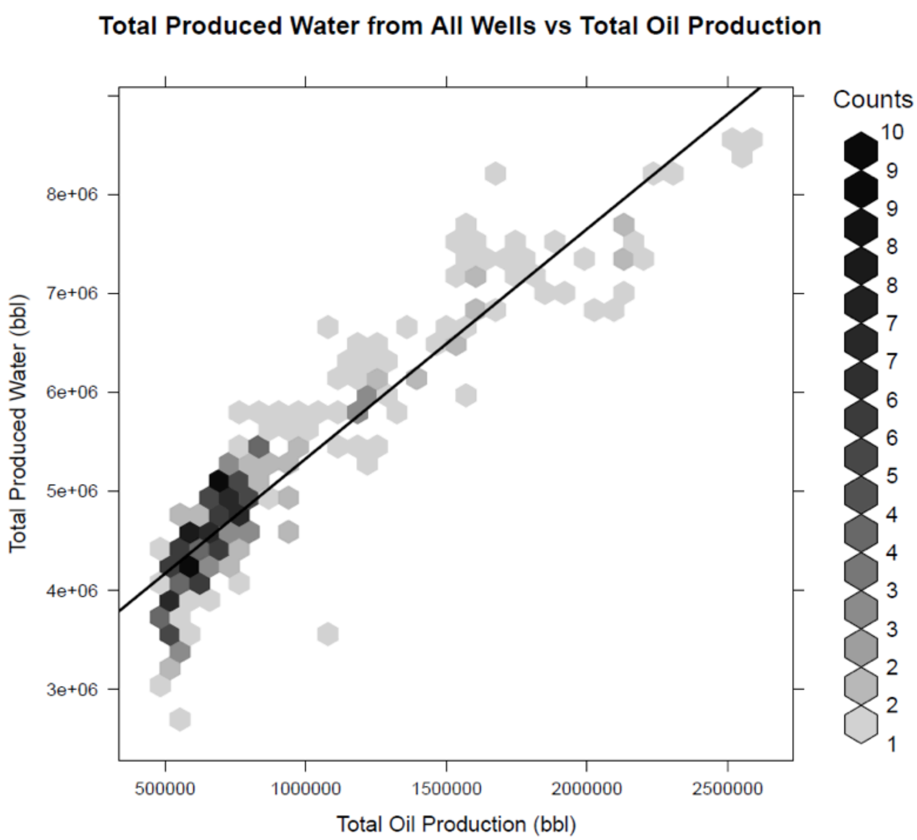

Figure 3. Regression to water balance data on ratio of produced water to oil production for all wells in the Uinta Basin in the 1994–2012 time period.

Overall, this analysis of past water balance data shows conventional oil and gas production is a net zero water user or very small water producer (producing approximately 0.16 ± 0.24 (at the 95% confidence interval) barrels of water per barrel of oil during the 2007–2013 time period).

Drilling Schedule Model

The largest source of uncertainty in predicting the environmental and economic impacts of oil and gas production in the Uinta Basin is estimating future drilling activity. Previous efforts looked at modeling drilling activity as a function of energy prices and prior drilling activity but had limited success at following actual drilling trends ($R^2 < 0.4$). However, in this quarter researchers have developed a model that accurately tracks with historical drilling trends over the 1978-2012 time period ($R^2 = 0.9$) as shown in Figure 4. The improvement is due to fitting to (1) the entire basin instead of each individual field, (2) wells drilled instead of the number of Applications for Permits to Drill (APDs) submitted, and (3) the total number of wells drilled instead of individual wells types (oil or gas). This improved model will be used with (1) EIA energy price forecasts and (2) randomly generated Geometric Brownian Motion (GBM) price paths to generate a range of predictions for drilling activity in the Uinta Basin.

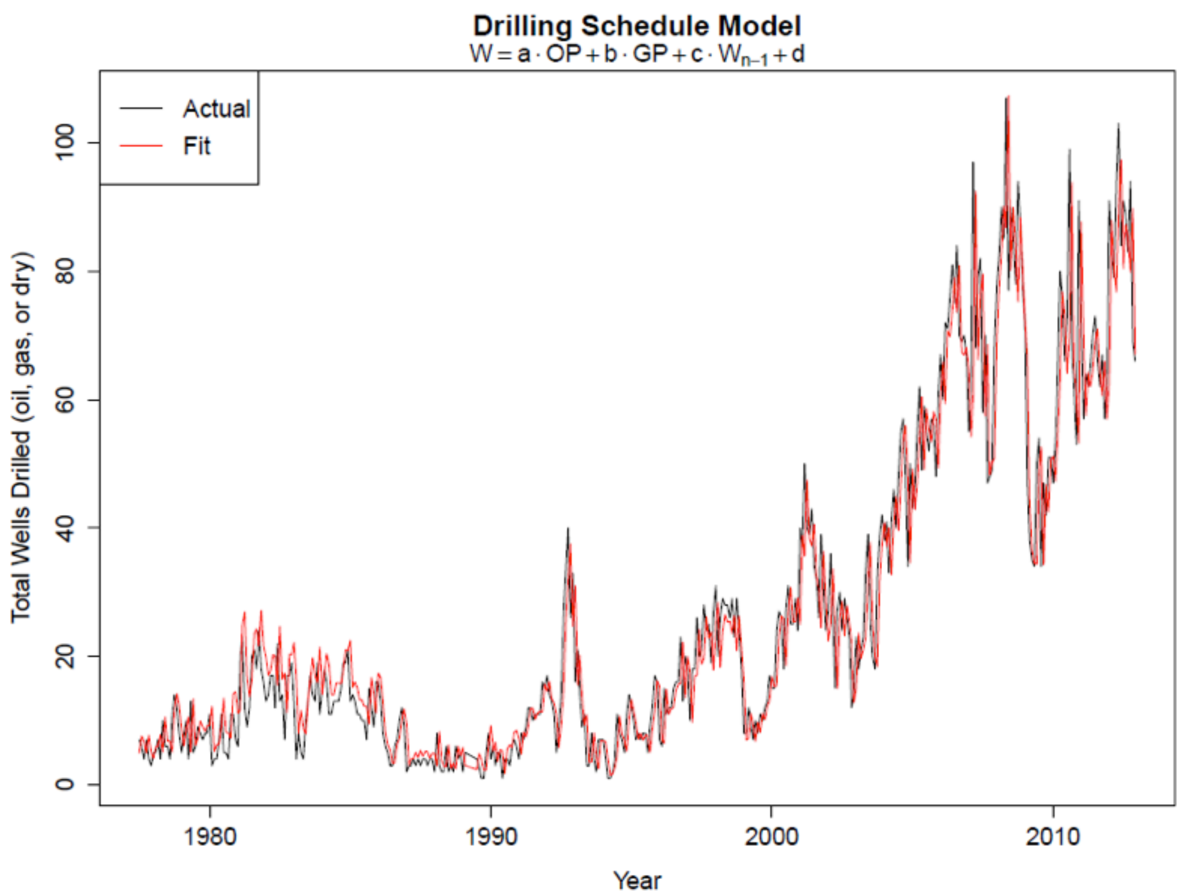

Figure 4. Drilling schedule model fit. Actual number of wells drilled in the Uinta Basin (oil wells, gas wells, or dry wells) is shown in black versus fitted predictions (red).

Centralized Modeling Framework

Finally, the project team revised the majority of the code (written in R) into a more centralized and user friendly format with one main driving script and a supporting text file for containing all modeling options. This revised code structure will be more user friendly and understandable to end users.

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

A summary of progress in this subtask is included with the Subtask 3.3 summary above.

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

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

Previously, the project team introduced a new strategy for capturing heating in rubblized oil shale beds using High Performance Computing (HPC) simulation tools. Instead of resolving every single piece of shale, they have incorporated a porous flow simulation, which accounts for an average bed porosity. In the past quarter, tested their new approach on a larger scale test geometry. This new domain is on a more realistic scale, as shown in Figure 5. Variable porosity from top to bottom, representing different particle distributions within the retorting bed, has been incorporated In this domain as depicted in Figure 6.

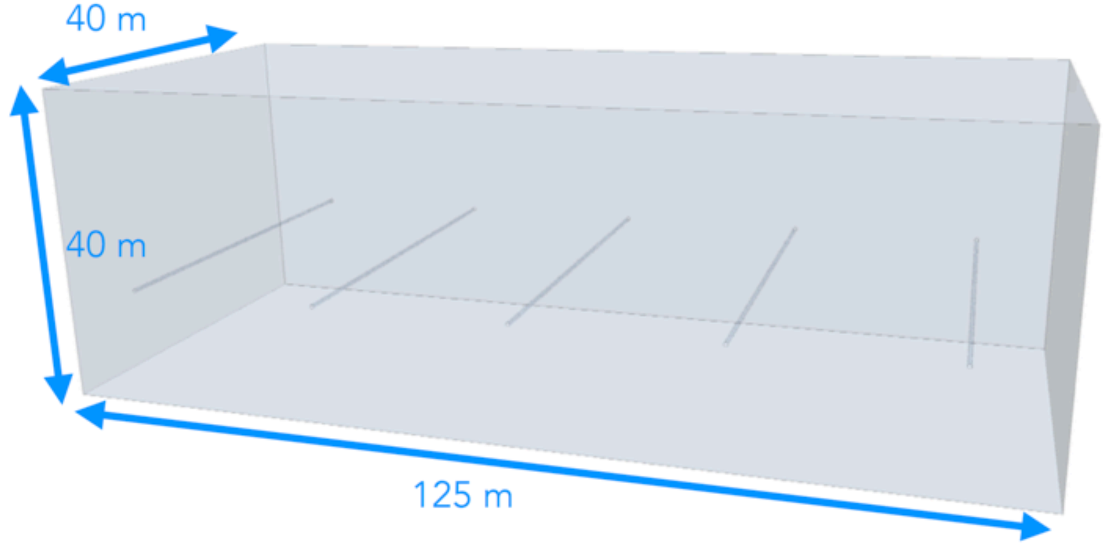

Figure 5. Porous media test domain.

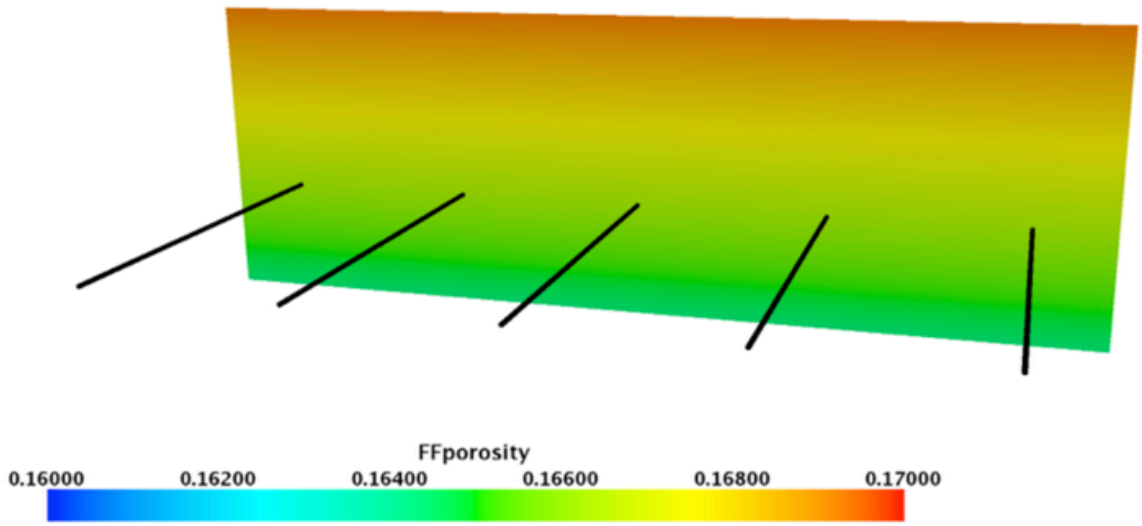

Figure 6. Variable porosity within our test domain.

As mentioned in the previous quarterly report, simulations resolving flow through porous media have become much more computationally expensive because of the short time scales that need to be resolved when producing oil and representing flow of oil through oil shale rock. These small time steps (on the order of 1e-3 seconds) required for computational stability have delayed the completion of any simulations in this quarter. Team members continue to improve their solution algorithm to achieve manageable computer time requirements to simulate realistic periods of time needed for retorting in rubblized oil shale beds.

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

A draft version of the final deliverable, a topical report on validation results for core-scale oil shale pyrolysis, was received in this quarter. An edited version of the report will be submitted as soon as it is completed.

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

The contract period was extended and additional funds were allocated to this project for the two milestones listed below. Both were completed this quarter as reported in the following summary.

- Perform experiments to resolve differences between Fletcher group & Deo group TGA data at 1 K/min
- Extend Chemical Percolation Devolatilization (CPD) model for oil shale to include additional chemical structure features specific to oil shale

There are two remaining deliverables for this project. A topical report is being written based on all of the data obtained in this project. The principal authors of the topical report are Dr. Fletcher and Dr. Pugmire. The journal paper on the CPD model application to oil shale will be finalized and sent to a journal for review. Current plans are to include the carbon balance and elemental compositions in the journal article (and certainly in the topical report).

Comparison of Oil Shale Pyrolysis Models

Efforts to obtain repeatable and reliable data at 0.25 K/min were unsuccessful. It is the opinion of team members that the accuracy of the thermocouples is insufficient for control at these heating rates. If the controller updates at 1 second intervals, the accuracy required would be 0.0042 K, which is quite unreasonable. Thus, there was no way to resolve the previously stated differences in the thermogravimetric analyzer (TGA) rate data obtained at Brigham Young University (BYU) and that reported by Dr. Deo's group at the University of Utah. Team members had a discussion with Dr. Alan Burnham, a reviewer on the papers by Hillier and Fletcher (Hillier, 2011; Hillier and Fletcher, 2011), about how these rates compared with his previous work at Lawrence Livermore National Laboratory. Dr. Burnham is satisfied that the BYU rates agree quite well with his published rates. The project team is therefore recommending using the BYU rates. A summary of these rates for the Utah Green River oil shales studied in this project was reported in a previous quarterly report and will appear in the topical report.

CPD Model

The extension of the CPD model to predict the pyrolysis behavior of oil shale was discussed in the previous quarterly report and will serve as the basis for a journal paper. This work was presented at the 34th Oil Shale Symposium by Dr. Fletcher. There was a lot of interest in this paper from several scientists, specifically Alan Burnham from American Shale Oil (AMSO) and Mohammad Amer from Monash University in Melbourne, Australia. Others were interested to know if the CPD-type approach could be applied to other oil shales. Dr. Pugmire's group has performed the nuclear magnetic resonance (NMR) analysis for the Estonian kukersite but not for shales from other parts of the world.

CPD Model vs. NMR Data

To better understand oil shale pyrolysis, team members looked for a way to track the aromaticity of the char (e.g. organic material left behind after pyrolysis). Throughout pyrolysis, the aromaticity of the carbons in the char increased from 0.2 to 0.8 (Fletcher et al., 2014). A balance was performed assuming that no new aromatic carbons are produced during pyrolysis. With this assumption, a simple mass balance of the aromatic carbons should predict the final amount in the char. With this approach, one can then see if any aliphatic carbons become aromatic in the experiment. Table 6 shows the elemental analyses of unreacted kerogen, tar, and light gas from the kerogen retort. Note that the tar composition comes from the literature for a similar sample.

Table 6. Elemental compositions of shale oil and pyrolysis products.

	Weight Fractions					
	Oxygen	Hydrogen	Carbon	Sulfur	Nitrogen	Carbon Aromaticity
Extracted Kerogen[1]	0.081	0.095	0.762	0.037	0.025	0.2
Tar[2]	0.013	0.114	0.851	0.007	0.018	0.19
Gas[3]	0.651	0.0478	0.273	0.0	0.0	0.0

[1] The composition for the extracted kerogen comes from Solum et al. (2014).
[2] The composition for the tar comes from a study done by Netzel and Miknis (1982).
[3] The composition of the gas comes from from Fletcher et al. (2014). The composition is determined based on the assumption that the "Other" portion of the light gases composition graph can be averaged as water.

A carbon balance for the amount of carbon that is left in the char was then performed using the yields of Fletcher et al. (2014) for Green River shale oil shown in Table 7.

Table 7. Final yields of the pyrolysis of shale oil.

	Char	Tar	Gas
Final Weight Fraction	0.2018	0.6557	0.1426

The carbon balance is shown in Equation (4):

$$C_{shale} = C_{tar} * f_{tar} + C_{gas} * f_{gas} + C_{char} * f_{char} \tag{4}$$

Everything in Equation (4) is known except for C_{char}, which is calculated to be 0.818.

A similar balance on aromatic carbon is shown in Equation (5), assuming that aromatic carbons are not created or destroyed in the retort. The only unknown in Equation (5) is $f_{a'char}$.

$$C_{shale} * f_{a'shale} = C_{tar} * f_{a'tar} * f_{tar} + C_{char} * f_{a'char} * f_{char} \tag{5}$$

The calculated value of $f_{a'char}$ is 0.281, but the measured value of $f_{a'char}$ is 0.81. This difference between the actual and calculated aromaticity shows that some carbons become aromatic as the reaction moves forward. Researchers thought of several possible explanations: (1) parts of the carbon matrix that have broken off can be reattached through a ring addition (Figure 7, top) or (2) the hydrogen could be scavenged from the remaining matrix, forming new double bonds that then form into aromatic regions (Figure 7, bottom).

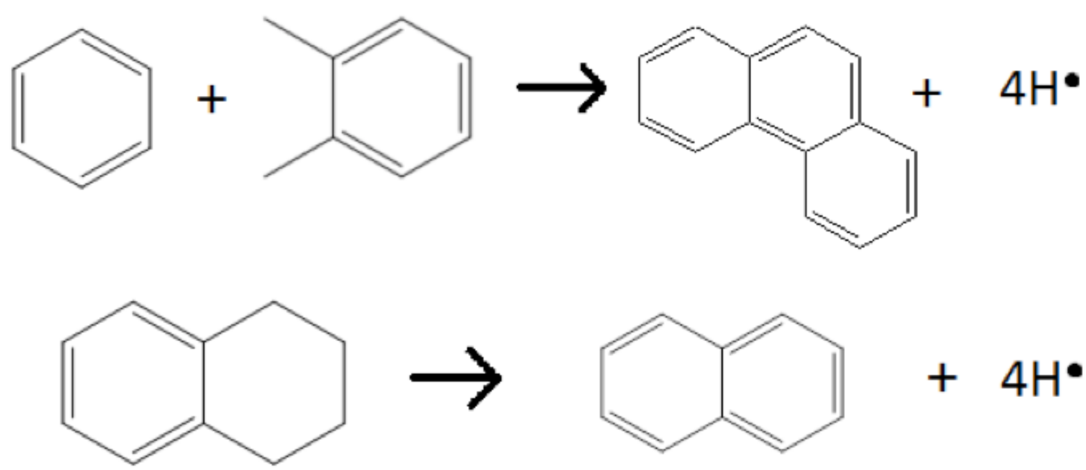

Figure 7. Two possible path ways to increase the aromaticity of the shale oil char.

Team members performed a thought experiment to verify the elemental composition of the tar. They assumed that the tar was 19% aromatic and 81% aliphatic by weight based on the percent aromaticity data of Fletcher et al. (2014). The aromatic fraction was assumed to have a carbon to hydrogen ratio of one (like benzene) and the aliphatic fraction was assumed to have the same carbon (C) to hydrogen (H) ratio as $C_{11}H_{25}$.

Then, the weight fraction of carbon in the aromatic fraction is calculated as follows:

$$\frac{Weight\ of\ Carbons}{Molecular\ Weight} = \frac{12.01}{12.01+1.008} = 0.923 \tag{6}$$

The weight fraction of carbon in the aliphatic fraction is calculated in a similar manner:

$$\frac{Weight\ of\ Carbons}{Molecular\ Weight} = \frac{11 \cdot 12.01}{11 \cdot 12.01+25 \cdot 1.008} = 0.84 \tag{7}$$

Therefore, a weighted average of the carbon content of the tar using these species as surrogates can be calculated as follows:

$$C_{tar} = f_{aromatic} * C_{aromatic} + f_{aliphatic} * C_{aliphatic} = .19 * .923 + .81 * .84 = 0.856 \tag{8}$$

The final carbon fraction of 0.856 is close to the carbon fraction in Netzel and Miknis (1982) as listed in Table 6. This thought experiment led the project team to believe that using the elemental compositions from the Netzel and Miknis paper is accurate enough for their model.

The present findings highlight the need to relook at changes in the char structure during pyrolysis. The reaction does not involve simple bridge-breaking mechanics as previously assumed for oil shale pyrolysis modeling. Instead, pyrolysis contains many reactions that link the char and that may contribute to which products are produced in the tar and the gas. Team members analyzed the amount of crosslinking in the CPD model, but that amount was negligible and would not add aromatic carbons anyway. Further work is needed to determine the exact mechanics of aromatic production and to model aromaticity. With such work, pyrolysis products and the chemical structure changes in the char can be more accurately predicted.

One of the questions that arose from this carbon aromaticity balance was the actual carbon content of the char samples from the experiments at BYU. The NMR samples were obtained from the University of Utah and were sent to Huffman Laboratories in Golden, Colorado for analysis. These analyses were paid for with BYU funds since DOE funding had ended. Results of the elemental char analyses are shown in Tables 7–9. Plots of carbon, hydrogen, and H to C ratio are shown in Figures 8 and 9. The project team is still analyzing these elemental composition data. However, the final measured carbon content of the char is 83 to 85 wt%, which is similar to the value of 81.8% calculated above.

Table 7. Elemental analysis of the GR1.9 chars.

T(°C)	C (wt% daf)	H (wt% daf)	N (wt% daf)	O (wt% daf)*	S (wt% daf)
300	78.85%	9.58%	2.90%	6.56%	2.11%
375	81.25%	9.96%	3.09%	3.73%	1.98%
410	80.38%	9.67%	3.13%	4.91%	1.93%
445	81.57%	9.65%	3.42%	3.51%	1.85%
495	85.16%	6.14%	5.42%	-1.28%	4.56%

Table 8. Elemental analysis of the GR2.9 chars.

T(°C)	C (wt% daf)	H (wt% daf)	N (wt% daf)	O (wt% daf)*	S (wt% daf)
425	80.44%	9.60%	3.05%	4.38%	2.52%
445	82.65%	9.30%	3.42%	2.58%	2.04%
475	83.40%	8.40%	4.04%	1.21%	2.95%
525	86.80%	3.98%	5.89%	-3.76%	7.09%

Table 9. Elemental analysis of the GR3.9 chars.

T(°C)	C (wt% daf)	H (wt% daf)	N (wt% daf)	O (wt% daf)*	S (wt% daf)
400	79.77%	9.45%	2.91%	5.19%	2.68%
434	80.84%	9.22%	3.12%	2.93%	3.89%
450	81.22%	8.61%	3.46%	3.44%	3.27%
460	82.64%	8.32%	3.78%	1.78%	3.48%
470	82.31%	7.89%	3.96%	1.84%	3.99%
490	82.50%	4.93%	5.22%	0.86%	6.49%
525	82.64%	3.77%	5.52%	1.25%	6.81%

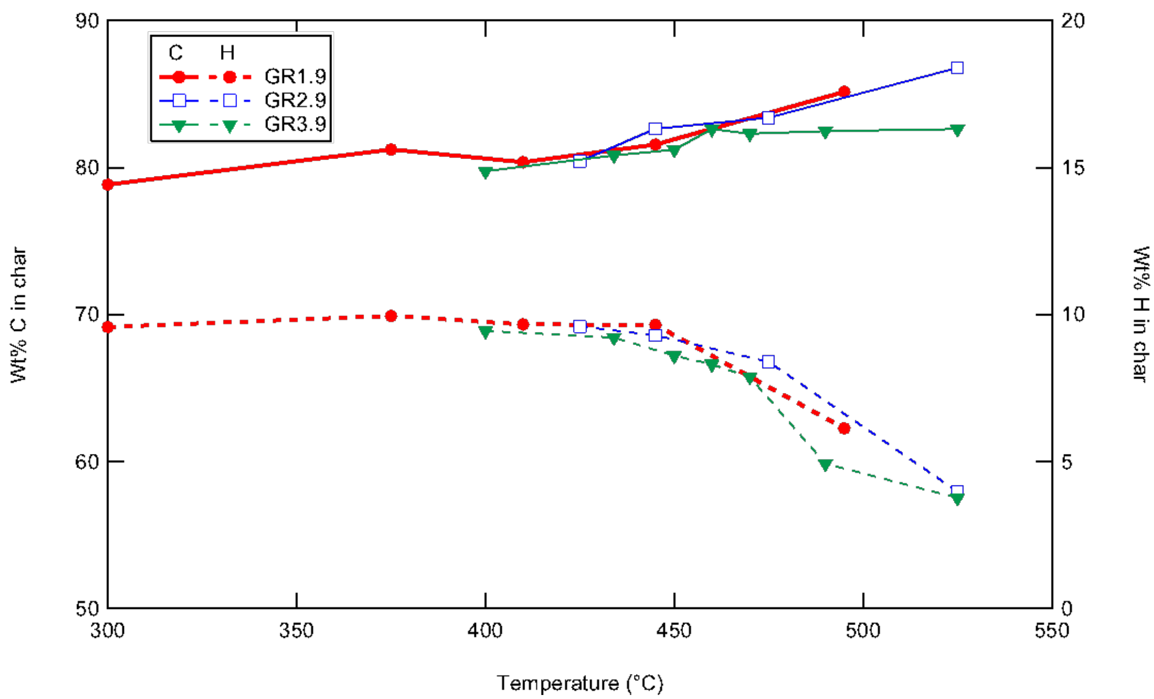

Figure 8. Carbon and hydrogen contents of the chars from the kerogen retort collected at different temperatures. The heating rate was 10 K/min for these experiments.

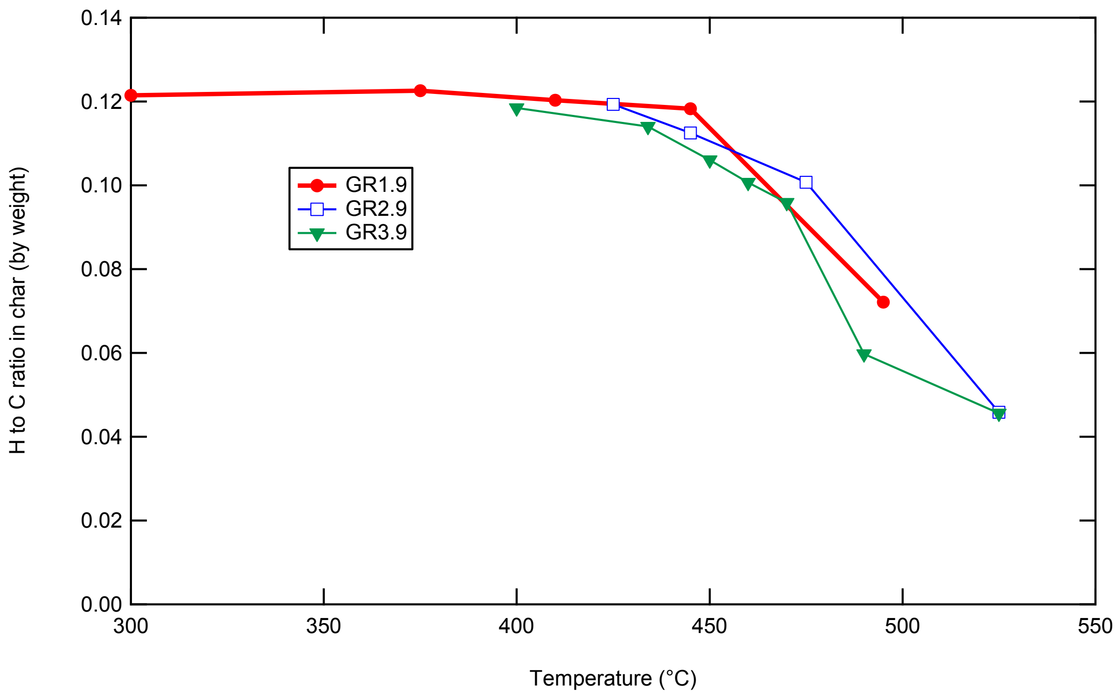

Figure 9. H to C ratios of the chars from the kerogen retort collected at different temperatures. The heating rate was 10 K/min for these experiments.

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

This project has been completed.

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

This project has been completed.

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

This project has been completed.

<u>Subtask 4.7 - Geomechanical Reservoir State (PI: John McLennan)</u>

No report received.

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

The project team is working on a topical report.

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

This project has been completed.

Task 5.0 - Environmental, Legal, Economic and Policy Framework

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

This project has been completed.

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

This project has been completed.

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

This project has been completed. A final topical report was sent to Mr. Robert Vagnetti on November 6, 2014.

6.0 – Economic and Policy Assessment of Domestic Unconventional Fuels Industry

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

This project has been completed.

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

This project has been completed

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

This project has been completed

7.0 – Strategic Alliance Reserve

Subtask 7.1 – Geomechanical Model (PI: John McLennan)

No report received.

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

Project has been terminated.

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

In the last quarter, researchers have continued to develop their HPC simulation tools for in-situ thermal treatment of oil shale. They completed their milestone of performing a simulation that incorporates kinetic compositional models as described below. They have also expanded their simulation domain, completed runs for three heating well arrangements, and presented their results at the 34th Oil Shale Symposium.

In the previous quarter, they introduced their newly developed simulation domain, which was more representative of the size of a commercial scale, in-situ retorting facility for oil shale. The simulation domain captures a 0.25 x 0.25 x 0.25 km^3 volume containing five heating wells, each with a 100 m long heating section. Most recently, the simulation domain has been modified to capture a retorting volume of 0.125 x 0.25 x 0.45 km^3, as shown in Figure 10. With this domain modification, heating wells with a 300 m long horizontal heating section can be captured. This domain has lateral periodic boundary conditions, shown in Figure 11. Therefore, it can be thought of as representing a small fraction of a realistic in-situ process, in which hundreds of horizontal wells are drilled next to one another. The heater temperature was assumed to be 675 K over the entire simulated time frame.

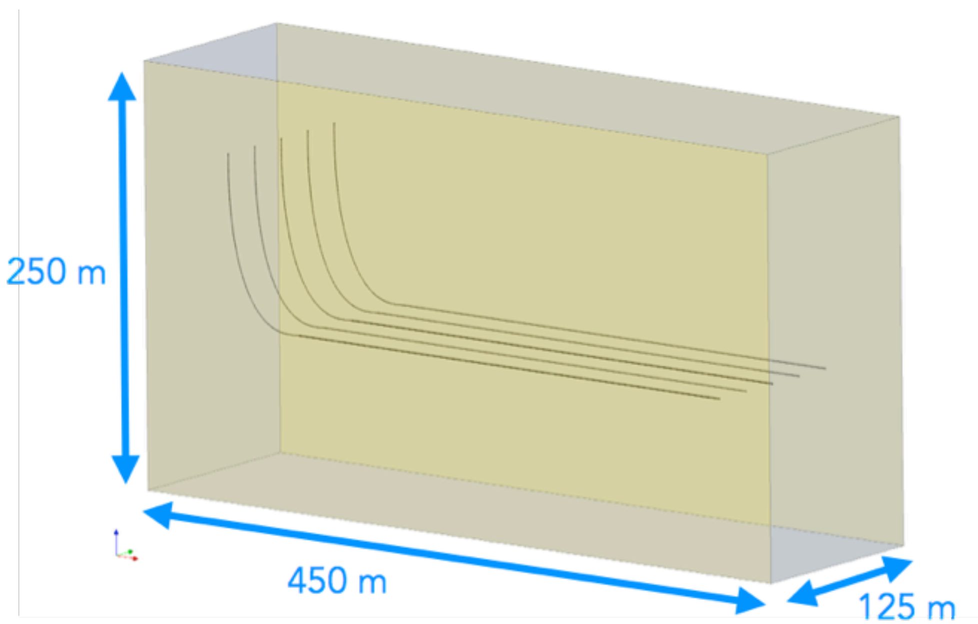

Figure 10. Modified simulation domain.

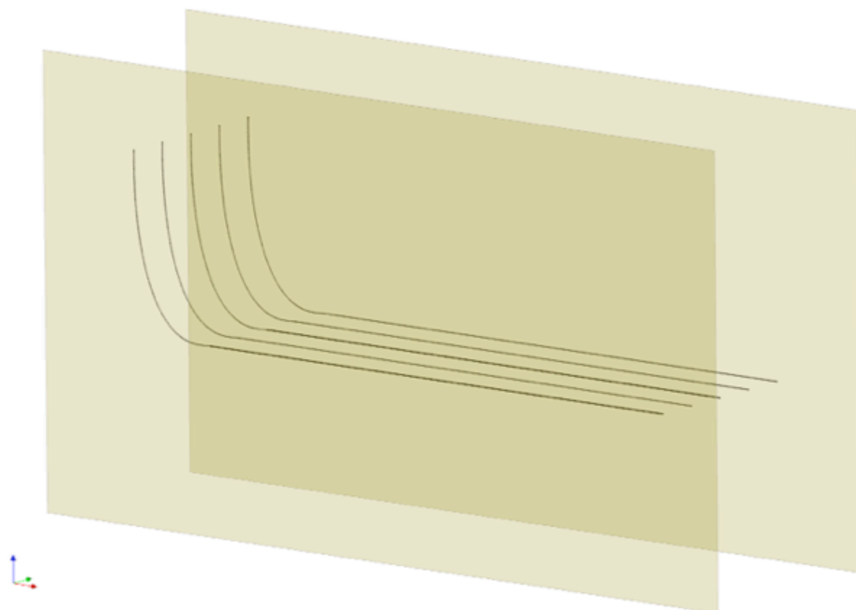

Figure 11. Lateral periodic boundary conditions.

Researchers have used this modified simulation domain to run three test scenarios with a target location in the Uinta Basin. They have used shale stratification information and physical properties obtained from Subtasks 4.3 and 4.8 as well as the open literature where appropriate. While the overall domain size remained constant for all three test scenarios, the number of wells and the well arrangement were changed. The first test case contained five heating wells spaced 25 m apart, as shown in Figure 12. The second test case, depicted in Figure 13, contained ten heating wells spaced 12.5 m apart. The last test case also contained ten heating wells. However, every second horizontal well was offset vertically 12.5 m to form a triangular pattern, as illustrated in Figure 14. Figure 15 shows a representative mesh with 50 million cells. The mesh for each case varied slightly in cell count because of the different well counts and arrangements.

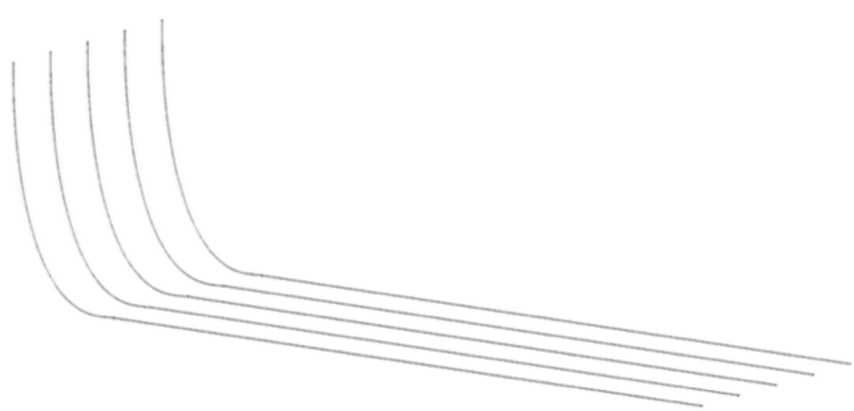

Figure 12. First test case scenario with 25 m lateral heater well spacing.

Figure 13. Second test case scenario with 12.5 m lateral heater well spacing.

Figure 14. Third test case scenario with 12.5 m lateral heater well spacing with every second well offset 12.5 m vertically to form a triangular pattern.

For the simulations, it was assumed that any oil produced was collected with kinetic parameters for oil yield taken from the results of Subtask 4.3. A simulation of each case was run long enough to capture heating over a two-year period. Figure 16 shows oil production over two years for the three cases. The required energy input needed to heat up oil shale to retorting temperature as well as oil yield and the resulting energy ratios are shown in Table 10. For this two-year heat up period, the energy in requirements exceed the energy out. However, in-situ processes are often considered on a time scale of five to seven years, so the simulations will be run out further in time to be more representative of an actual process. Results at longer times will be discussed in subsequent quarters.

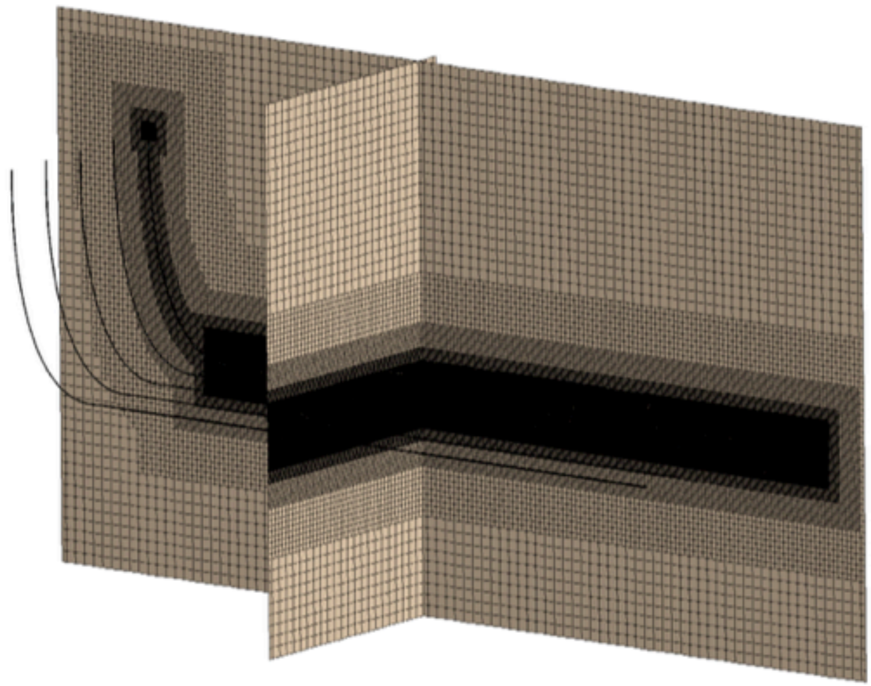

Figure 15. Representative mesh with about 50 million computational cells.

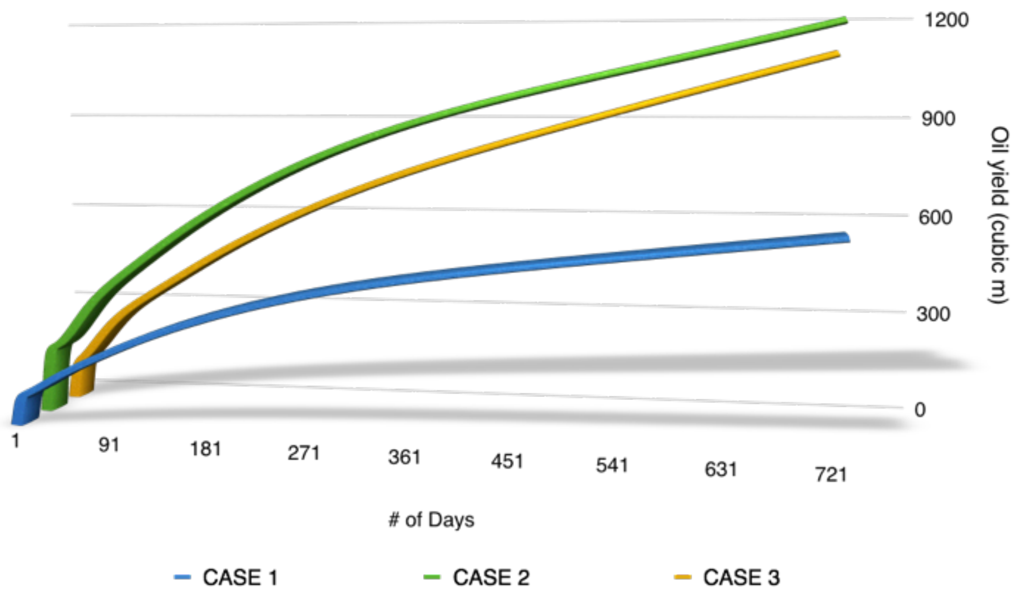

Figure 16. Oil production for all three cases after about two years of heating.

Table 10. Energy ratios for all three cases after two years of heating.

	Energy In ($x10^6$) (kWh)	Oil Yield (m^3)	Oil equivalent Energy Out ($x10^6$)(kWh)	NG equivalent Energy Out ($x10^6$)(kWh)	Energy In/ Energy Out
Case 1	13.9	592	6.33	6.84	2.03 - 2.20
Case 2	27.3	1,175	12.6	13.6	2.00 - 2.17
Case 3	43.2	1,120	12.0	12.9	3.35 - 3.60

These current results were presented at the 34th Oil Shale Symposium in October 2014. A copy of the presentation is included as Appendix A of this report.

CONCLUSIONS

Two topical reports were completed during this quarter. The Subtask 4.2 topical report, Reservoir Simulation of Reactive Transport Processes, is in draft form and will be submitted to DOE in November 2013. The Subtask 5.3 topical report, Policy and Economic Issues Associated with Using Simulation to Assess Environmental Impacts, was submitted to Mr. Robert Vagnetti on November 6, 2014. Subtask 3 research progressed with the refining of information on emission factors associated with natural gas production and processing, the addition of a water balance for conventional oil and gas development, the improvement of the conventional oil and gas drilling schedule model, and code revisions in the basin-scale model to make it more user-friendly. In Subtask 4.3, researchers reconciled TGA data from low heating rate oil shale pyrolysis experiments with data previously published by Alan Burnham. They also continued development of the CPD model for applications to oil shale kerogen pyrolysis. Researchers in Subtasks 4.1 and 7.3 used HPC tools to simulate length and time scales more commensurate with a commercial-scale operation.

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

Baseline Reporting Quarter - PHASE II	Yr. 4								Yr. 5			
	Q13		Q14		Q15		Q16 - REVISED		**Q17**		Q18	
	10/01/12 - 12/31/12		01/01/13 - 03/31/13		04/01/13 - 06/30/13		07/01/13 - 09/30/13		**10/01/13 - 12/31/13**		01/01/14 - 03/31/14	
	Q13	**Total**	Q14	**Total**	Q15	**Total**	Q16	**Total**	Q17	**Total**	Q18	**Total**
Baseline Cost Plan												
Federal Share	146,824	**5,235,073**	146,824	**5,381,897**	146,824	**5,528,721**	-471,238	**5,057,483**	157,250	**5,214,733**	157,250	**5,371,983**
Non-Federal Share	36,705	**1,306,563**	36,705	**1,343,268**	36,705	**1,379,973**	-211,982	**1,167,991**	53,484	**1,221,475**	53,484	**1,274,959**
Total Planned	183,529	**6,541,636**	183,529	**6,725,165**	183,529	**6,908,694**	-683,220	**6,225,474**	210,734	**6,436,208**	210,734	**6,646,942**
Actual Incurred Cost												
Federal Share	128,349	**4,485,377**	180,613	**4,665,990**	233,732	**4,899,722**	157,761	**5,057,483**	113,187	**5,170,670**	148,251	**5,318,921**
Non-Federal Share	79,871	**1,051,976**	62,354	**1,114,330**	51,708	**1,166,038**	1,953	**1,167,991**	66,131	**1,234,122**	48,378	**1,282,500**
Total Incurred Costs	208,220	**5,537,353**	242,967	**5,780,320**	285,440	**6,065,760**	159,714	**6,225,474**	179,318	**6,404,792**	196,629	**6,601,421**
Variance												
Federal Share	18,475	**749,696**	-33,789	**715,907**	-86,908	**628,999**	-628,999	**0**	44,063	**44,063**	8,999	**53,062**
Non-Federal Share	-43,166	**254,587**	-25,649	**228,938**	-15,003	**213,935**	-213,935	**0**	-12,647	**-12,647**	5,106	**-7,541**
Total Variance	-24,691	**1,004,283**	-59,438	**944,845**	-101,911	**842,934**	-842,934	**0**	31,416	**31,416**	14,105	**45,521**

Baseline Reporting Quarter - PHASE II	Yr. 5				Yr. 6							
	Q19		**Q20 - REVISED BUDGET**		Q21		Q22		Q23		Q24	
	04/01/14 - 06/30/14		**07/01/14 - 09/30/14**		10/01/14 - 12/31/14		01/01/14 - 03/31/15		04/01/15 - 06/30/15		07/01/15 - 09/30/15	
	Q19	**Total**	Q20	**Total**	Q19	**Total**	Q20	**Total**	Q19	**Total**	Q20	**Total**
Baseline Cost Plan												
Federal Share	157,250	**5,529,233**	80,000	**5,609,233**	35,000	**5,644,233**	10,000	**5,654,233**	4,000	**5,658,233**	4,282	**5,662,515**
Non-Federal Share	53,484	**1,328,443**	44,136	**1,372,579**	30,000	**1,402,579**	8,000	**1,410,579**	3,000	**1,413,579**	2,300	**1,415,879**
Total Planned	210,734	**6,857,676**	124,136	**6,981,812**	65,000	**7,046,812**	18,000	**7,064,812**	7,000	**7,071,812**	1,700	**7,078,394**
Actual Incurred Cost												
Federal Share	147,582	**5,466,503**	86,384	**5,552,887**		**0**		**0**		**0**		**0**
Non-Federal Share	46,472	**1,328,971**	38,582	**1,367,554**		**0**		**0**		**0**		**0**
Total Incurred Costs	194,053	**6,795,474**	124,966	**6,920,441**	0	**0**	0	**0**		**0**	0	**0**
Variance												
Federal Share	9,668	**62,730**	-6,384	**56,346**	35,000	**5,644,233**	10,000	**5,654,233**	4,000	**5,658,233**	4,282	**5,662,515**
Non-Federal Share	7,012	**-528**	5,554	**5,025**	30,000	**1,402,579**	8,000	**1,410,579**	3,000	**1,413,579**	2,300	**1,415,879**
Total Variance	16,681	**62,202**	-830	**61,371**	65,000	**7,046,812**	18,000	**7,064,812**	7,000	**7,071,812**	1,700	**7,078,394**

Note: Baseline Cost Plan adjusted in Q20 to reflect second NCE projections.

MILESTONE STATUS

ID	Title/Description	Planned Completion Date	Actual Completion Date	Milestone Status
1.0	Project Management			
2.0	Technology Transfer and Outreach			
	Advisory board meeting	Jun-13	N/A	Decision has been made to disband EAB
	Hold final project review meeting	Jun-13		NCE will delay this meeting until 2014
3.0	Clean Oil Shale & Oil Sands Utilization with CO2 Management			
3.1	Lifecycle greenhouse gas analysis of conventional oil & gas development in the Uinta Basin			
	Complete modules in CLEAR CO2 emissions from conventional oil & gas development in the Uinta Basin	Nov-14		Milestone date has been changed to reflect new project timelines
3.2	Flameless oxy-gas process heaters for efficient CO2 capture			
	Preliminary report detailing results of skeletal validation/uncertainty quantification analysis of oxy-gas combustion system	Sep-12	Oct-12	Report attached as appendix to Oct. 2012 quarterly report
3.3	Development of oil & gas production modules for CLEAR			
	Develop preliminary modules in CLEAR for conventional oil & gas development & produced water management in Uinta Basin	Oct-11	Dec-11	Discussed in Jan. 2012 quarterly report
3.4	V/UQ analysis of basin scale CLEAR assessment tool			
	Develop a first generation methodology for doing V/UQ analysis	Oct-11	Nov-11	Discussed in Jan. 2012 quarterly report
	Demonstrate full functionality of V/UQ methodology for conventional oil development in Uinta Basin	Nov-13	Apr-14	Demonstration delayed until first quarter of 2014
	Demonstrate full functionality for conventional & unconventional oil development in Uinta Basin	Mar-14	Jun-14	Discussed in this quarterly report
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	Mar-12	Discussed in April 2012 quarterly report
4.2	Reservoir simulation of reactive transport processes			
	Incorporate kinetic & composition models into both commercial & new reactive transport models	Dec-11	Dec-11	Discussed in Jan. & July 2012 quarterly reports
	Complete examination of pore-level change models & their impact on production processes in both commercial & new reactive transport models	Jun-12	Jun-12	Discussed in July 2012 quarterly report
4.3	Multiscale thermal processes			
	Complete thermogravimetric analyses experiments of oil shale utilizing fresh “standard” core	Sep-11	Sep-11	Discussed in Oct. 2011 quarterly report
	Complete core sample pyrolysis at various pressures & analyze product bulk properties & composition	Dec-11	Sep-12	Discussed in Oct. 2012 quarterly report
	Collection & chemical analysis of condensable pyrolysis products from demineralized kerogen	May-12	Sep-12	Discussed in Oct. 2012 quarterly report
	Complete model to account for heat & mass transfer effects in predicting product yields & compositions	Jun-12	Jun-12	Discussed in July 2012 quarterly report
	Perform experiments to resolve differences between Fletcher group & Deo group TGA data at 1 K/min	Jul-14	Sep-14	Discussed in this quarterly report
	Extend CPD model for oil shale to include additional chemical structure features specific to oil shale	Jul-14	Sep-14	Discussed in this quarterly report
4.5	In situ pore physics			
	Complete pore network structures & permeability calculations of Skyline 16 core (directional/anisotropic, mineral zones) for various loading conditions, pyrolysis temperatures, & heating rates	Mar-12	Mar-12	Discussed in April 2012 quarterly report; PI dropped loading condition as variable
4.6	Atomistic modeling of oil shale kerogens & oil sand asphaltenes			
	Complete web-based repository of 3D models of Uinta Basin kerogens, asphaltenes, & complete systems (organic & inorganic materials)	Dec-11	Dec-11	Discussed in Jan. 2012 quarterly report
4.7	Geomechanical reservoir state			
	Complete high-pressure, high-temperature vessel & ancillary flow system design & fabrication	Sep-11	Sep-11	Discussed in Oct. 2011 quarterly report

ID	Title/Description	Planned Completion Date	Actual Completion Date	Milestone Status
	Complete experimental matrix	Mar-14	May-14	Report sent to R. Vagnetti on 27 May 2014
	Complete thermophysical & geomechanical property data analysis & validation	Dec-14		Due date has been revised to reflect status of expts.
4.8	Developing a predictive geologic model of the Green River oil shale, Uinta Basin			
	Detailed sedimentologic & stratigraphic analysis of three cores &, if time permits, a fourth core	Dec-12	Dec-12	Discussed Jan. 2013 quarterly report
	Detailed mineralogic & geochemical analysis of same cores	Dec-12	Dec-12	Discussed Jan. 2013 quarterly report
4.9	Experimental characterization of oil shales & kerogens			
	Characterization of bitumen and kerogen samples from standard core	Jan-12	Feb-12	Email sent to R. Vagnetti on Feb. 6, 2012 & discussed in April 2012 quarterly report
	Development of a structural model of kerogen & bitumen	Jun-12	Jun-12	Discussed in July 2012 quarterly report
5	Environmental, legal, economic, & policy framework			
5.1	Models for addressing cross-jurisdictional resource management			
	Identify case studies for assessment of multi-jurisdictional resource management models & evaluation of utility of models in context of oil shale & sands development	Jun-11	Jul-11	Discussed in Oct. 2011 quarterly report
5.2	Conjunctive management of surface & groundwater resources			
	Complete research on conjunctive surface water & groundwater management in Utah, gaps in its regulation, & lessons that can be learned from existing conjunctive water management programs in other states	Aug-11	Aug-11	Discussed in Oct. 2011 quarterly report
5.3	Policy & economic issues associated with using simulation to assess environmental impacts			
	White paper describing existing judicial & agency approaches for estimating error in simulation methodologies used in context of environmental risk assessment and impacts analysis	Dec-12	Dec-12	Submitted with Jan. 2103 quarterly report

ID	Title/Description	Planned Completion Date	Actual Completion Date	Milestone Status
6	Economic & policy assessment of domestic unconventional fuels industry			
6.1	Engineering process models for economic impact analysis			
	Upload all models used & data collected to repository	Oct-12	Aug-13	All models/data have been uploaded to the ICSE website
7	Strategic Alliance Reserve			
	Conduct initial screening of proposed Strategic Alliance applications	Mar-11	Mar-11	
	Complete review and selection of Strategic Alliance applications	Jun-11	Jul-11	Discussed in Oct. 2011 quarterly report
	Implement new Strategic Alliance research tasks	Sep-11	Sep-11	Discussed in Oct. 2011 quarterly report
7.1	Geomechanical model			
	Make experimental recommendations	Aug-13	Aug-13	Discussed in this quarterly report
	Infer permeability-porosity-temperature relationships, develop model that can be used by other subtasks	Dec-14		Due date has been revised to reflect status of expts.
	Basic reservoir simulations to account for thermal front propagation	Mar-15		Due date has been revised to reflect status of expts.
	Evaluation of flow mechanics	Mar-15		Due date has been revised to reflect status of expts.
7.2	Kinetic compositional models & thermal reservoir simulators			Project has been terminated
	Incorporate chemical kinetics into thermal reservoir simulators	Jun-12	Jun-12	Discussed in July 2012 quarterly report
7.3	Rubblized bed HPC simulations			
	Collect background knowledge from AMSO about characteristics & operation of heated wells	Jun-12	Jun-12	Discussed in July 2102 quarterly report
	Perform generation 1 simulation - DEM, CFD & thermal analysis of characteristic section of AMSO rubblized bed	Sep-12	Sep-12	Discussed in Oct. 2012 quarterly report
	Perform generation 2 simulation that incorporates kinetic compositional models from subtask 7.2 and/or AMSO	Sep-14	Sep-14	Discussed in this quarterly report

NOTEWORTHY ACCOMPLISHMENTS

Researchers from Subtasks 4.3 and 7.3 presented their work at the 34th Oil Shale Symposium in Golden, CO in October 2014. Additionally, the Utah Department of Air Quality has funded a project that will leverage the work that has been completed under Subtasks 3.3. and 3.4.

PROBLEMS OR DELAYS

No report was received for Subtasks 4.8 and 7.1, so their current status is unclear.

RECENT AND UPCOMING PRESENTATIONS/PUBLICATIONS

Pugmire, R. J., Fletcher, T. H., Hillier, J., Solum, M., Mayne, C. & Orendt, A. (2013, October). Detailed characterization and pyrolysis of shale, kerogen, kerogen chars, bitumen, and light gases from a Green River oil shale core. Paper presented at the 33rd Oil Shale Symposium, Golden, CO, October 14-16, 2013.

Fletcher, T. H., Gillis, R., Adams, J., Hall, T., Mayne, C. L., Solum, M.S. & Pugmire, R. J. (2013, October). Characterization of pyrolysis products from a Utah Green River oil shale by ^{13}C NMR, GC/MS, and FTIR. Paper presented at the 33rd Oil Shale Symposium, Golden, CO, October 14-16, 2013.

Wilkey, J., Spinti, J., Ring, T., Hogue, M. & Kelly, K. (2013, October). Economic assessment of oil shale development scenarios in the Uinta Basin. Paper presented at the 33rd Oil Shale Symposium, Golden, CO, October 14-16, 2013.

Hillier, J. L., Fletcher, T. H., Solum, M. S. & Pugmire, R. J. (2013, October). Characterization of macromolecular structure of pyrolysis products from a Colorado Green River oil shale. Accepted, *Industrial and Engineering Chemistry Research*. dx.doi.org/10.1021/ie402070s

Birgenheier, L. & Vanden Berg, M. (n.d.). Facies, stratigraphic architecture, and lake evolution of the oil shale bearing Green River Formation, eastern Uinta Basin, Utah. To be published in Smith, M. and Gierlowski-Kordesch, E. (Eds.). *Stratigraphy and limnogeology of the Eocene Green River Formation*, Springer.

Solum, M. S., Mayne, C. L., Orendt, A. M., Pugmire, R. J., Hall, T., Fletcher, T. H. (2014). Characterization of macromolecular structure elements from a Green River oil shale-(I. Extracts). Submitted to *Energy and Fuels, 28*, 453-465. dx.doi.org/10.1021/ef401918u,

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Hradisky, M., Smith, P. J., Burnham, A. K. (2014, March). STAR-CCM+ high performance computing simulations of oil shale retorting system using co-simulation. Presented at the STAR Global Conference, Vienna, Austria. March 2014.

Barfuss, D. C., Fletcher, T. H. Fletcher and Pugmire, R. J. (2014, October). Modeling oil shale pyrolysis using the Chemical Percolation Devolatilization model. Abstract submitted for a presentation at the 35th Oil Shale Symposium, Golden, CO, October 13-15, 2014.

Hardisky, M. and Smith, P. J. (2014, October). Evaluation of well spacing and arrangement for in-situ thermal treatment of oil shale using HPC simulation tools. Abstract submitted for a presentation at the 35th Oil Shale Symposium, Golden, CO, October 13-15, 2014.

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Appendix A. Evaluation of Well Spacing and Arrangement for In-situ Thermal Treatment of Oil Shale Using HPC Simulation Tools. Presentation given by Dr. Michal Hradisky at the 34th Oil Shale Symposium in Golden, CO, October 13-15, 2014.

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