Oil & Natural Gas Technology

DOE Award No.: DE-FE0001243

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

Quarterly Progress Report (April – June 2010)

Submitted by:
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155 S. 1452 E. Room 380
Salt Lake City, Utah 84112

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

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Office of Fossil Energy

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EXECUTIVE SUMMARY

The Clean and Secure Energy from Domestic Oil Shale and Oil Sands Resources program is part of the research agenda of the Institute for Clean and Secure Energy (ICSE) at the University of Utah. In this quarter, the Clean and Secure Energy program continued its efforts to enhance the dialogue between ICSE and industry and to engage in academic and public outreach/education efforts by holding the annual ICSE Industrial Advisory Board Meeting, presenting ICSE research at the 2010 University of Utah Unconventional Fuels Conference, continuing the expansion of the ICSE Digital Repository in support of ongoing ICSE research activities and of dissemination of work completed by ICSE researchers, evaluating and integrating map usage tracking software for visitors to the Interactive Map, and continuing work on the new ICSE website.

In Task 3.0, ICSE researchers have completed their data gathering on the potential of oxy-fuel for CO_2 capture in refining and included other greenhouse gases (GHGs) such CH_4 and N_2O in the analysis. For oxy-gas simulation, researchers are refocusing their efforts on a recently released oxy-gas dataset from the International Flame Research Foundation due to repeated problems in performing simulations of the OXYFLAM experiments.

In Task 4.0, ICSE researchers were able to obtain a 4-inch oil shale core sample from nearly the entire oil shale zone (Parachute Creek Member) at a drilling site on private lands owned by Oil Shale Exploration Company in the eastern Uinta Basin of Utah. Future research in this task will focus on this fresh core sample to better integrate research among all subtasks at all scales. The Subtask 4.1 team demonstrated the ability of Star-CCM+ to handle large (on the order of a thousand bodies) geometry operations and selected it in place of Gambit for geometry handling. EDEM simulations are still used to create randomly-spaced pieces of shale and to provide geometry data, which are now directly post-processed in Matlab to create a java script to be used with Star-CCM+. This new capability was used to perform preliminary simulations of a simple ECOSHALE capsule geometry. The Subtask 4.2 team used a fractional factorial experimental design to expose the parameters with greatest impact on the ultimate recovery of oil from an in-situ oil shale production process. Using a reaction mechanism with seven pseudo components, four significant parameters were determined. These four significant parameters were explored further with a full factorial experimental design to create a response surface model. Researchers in Subtask 4.3 calculated the kinetic parameters of thermal decomposition (pyrolysis) of fine powdered Green River oil shale samples in thermal gravimetric analyzer experiments using various kinetic models. The results were compared with parameters from model-free advanced isocoversion models, and the isoconversional models appear best suited to describe the data. The Subtask 4.4 team completed six hydrous experiments at various conditions and will send the water samples out for analyses to measure organic concentrations. In Subtask 4.5, the team performed detailed 3-D imaging of oil shale core samples after pyrolysis at three reaction temperatures (300˚C, 350˚C, and 400˚C) to establish the pore structure of the core after reaction using high resolution X-ray microtomography for imaging (~ 5 micron voxel resolution). Some of the pore space created during pyrolysis was clearly visible at this resolution and it was possible to distinguish between the pyrolyzed oil shale and the host shale rock. ISCE researchers in Subtask 4.6 switched from kerogen modeling to modeling of the asphaltene structures present in oil sands. This work mirrors that previously done on the kerogen model. Work also began on modeling of inorganic matter in order to study interactions between the organic kerogen/asphaltene models and the inorganic material. Team members now have a 3-D structure of illite (an aluminum silicate clay structure) ready to use in these studies.

In Task 5.0, ICSE researchers focused primarily on issues related to wildlife and plants, on access to oil shale and oil sands resources, and on water resources and produced water, including analysis of historic water law insofar as it relates to water rights that vested prior to enactment of the current Utah water code. Among other topics, researchers reviewed (and will continue to monitor) draft federal legislation regarding wildlife migration corridors, the most recent Endangered Species Act listing of plants found on portions of the Mahogany Outcrop within Colorado, and Wyoming statutory and case law regarding water produced during natural gas extraction.

In Task 6.0, the research team built models for in-situ and ex-situ extraction of oil sands, in-situ and ex-situ extraction of oil shale, and in-situ extraction of heavy oil from the North Slope of Alaska. These models are included as a supplement to this quarterly report in an Excel file. The project team also drafted two sections of the Market Assessment. One is a preliminary version of the section addressing differences between the United States and Canada in terms of taxes and royalties levied on oil sands production as well as downstream and marketing challenges facing oil sands development. The other is an assessment of impacts to revenue corresponding to each scenario listed above. To complete this assessment, the project team gathered data and created models for implementing the chosen methodology to carry out a sensitivity analysis on the monthly revenue for each scenario.

PROGRESS, RESULTS, AND DISCUSSION

Task 1.0 - Project Management and Planning

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

Task 2.0 -Technology Transfer and Outreach

This task concentrates efforts on enhancing the dialogue between ICSE and industry and on engaging in academic and public outreach/education efforts. Milestones reached during this quarter included holding the annual ICSE Industrial Advisory Board Meeting, presenting ICSE research at the 2010 University of Utah Unconventional Fuels Conference, continuing the expansion of the ICSE Digital Repository in support of ongoing ICSE research activities and of dissemination of work completed by ICSE researchers, and evaluating and integrating map usage tracking software for visitors to the Interactive Map. Although not a milestone, significant progress was also made on the new ICSE website during this quarter.

The Industrial Advisory Board Meeting was held on April 27, 2010; the agenda for that meeting is included in Appendix A. Board members in attendance were Ian Andrews (Pacificorp), Spencer Eccles, Jr. (Utah Governor’s Office of Economic Development), James Holtkamp (Holland & Hart, LLP) Sho Kobayashi (Praxair), John Marion (Alstom Power), Dianne Nielson (Utah Governor’s Office), Laura Nelson (Red Leaf Resources), Mark Raymond (Uintah County) Kevin Shurtleff (USTAR & Mountain West Energy), Joseph Strakey (NETL), David Tabet (Utah Geological Survey), Andrew Wolfsberg (Los Alamos National Laboratory). Substantive feedback was received from members of the Board and draft recommendations based on that input are being finalized. These recommendations will be presented to ICSE researchers next quarter.

ICSE sponsored the University of Utah Unconventional Fuels Conference on April 28, 2010; an agenda for the conference is included in Appendix B. In contrast to previous years, this year’s conference offered a broader consideration of unconventional fuels, examining in-situ production of coal as well as oil shale and oil sands. The conference featured presentations, a poster session highlighting ICSE research, and an oil shale core workshop hosted by the Utah Geological Survey. The conference drew local and national media attention, in large part due to remarks offered at the conference by Steve Black, Counselor to Secretary of Interior Salazar. The conference continues to enjoy strong attendance among both new and repeat attendees.

In other technology transfer and outreach activities during this quarter, Terrance Davis, the Institute's Web Applications Programmer, completed a necessary upgrade of the DSpace database (the platform used for the ICSE Digital Repository). The database upgrade consisted of a complete data migration and a rewrite of DSpace code relating to data access. The upgrade has resulted in a notable speed increase to the repository's performance.

The Institute Librarian, Wendy Ajax, has continued to work on developing the ICSE public and private Scholarship collections housed in the ICSE Digital Repository. These collections include journal articles, conference presentations and publications, and reports produced by ICSE researchers. She also has created a public Management Collection in the repository to house award portfolios, quarterly reports, and other relevant management documents. The Institute Librarian has continued to work with ICSE researchers on maintaining the Digital Repository's private collections, which have been developed for the following specific research groups: Carbon Mineralization; Chemical Looping Combustion; Coal Gasification; DQMOM; Environmental, Legal, & Policy Framework for Fossil Energy Development; In-situ Thermal Processing of Oil Shale/Sands, Market Assessment of Heavy Oil, Oil Sands, & Oil Shale Resources; Oxy-fuel Combustion; Underground Coal Thermal Treatment; Verification, Validation, and Uncertainty Quantification. These collections include relevant documents that inform and support the research of the groups.

Work on the Interactive Map this past quarter focused on tracking map usage. To maximize the utility of the map, the Institute GIS Applications Developer, Michelle Kline, has implemented a map usage tracking system that logs information about each visit to the map. Each time an end user visits the map, basic information about the user is recorded. Each end user's network URL, internet service provider and country are recorded. This basic information is tracked using StatCounter, a common, free website statistics tracking software package. In addition to this basic information, more specific information is recorded using custom built software housed on the map server. This custom software records the actions the user takes while visiting the map, as well as what data layers the user views. The purpose of gathering and analyzing the statistical usage of the map is to be able to determine what data is of most interest to end users and to develop the utilities of the map accordingly.

Finally, significant work was completed on developing a more integrated ICSE website. An Institute Webmaster, Andrew Morgenegg, was hired to work with the Graphic Designer, Adam Tayor, to redesign and code the ICSE website, which will be completed next quarter.

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

Subtask 3.1 – Macroscale CO_2 Analysis

During this quarter, the project team completed their data gathering on the potential of oxy-fuel for CO_2 capture in refining and included other greenhouse gases (GHGs) such CH_4 and N_2O in the analysis. In spite of the higher global-warming potential of CH_4 and its potential release during transport of natural gas required for firing the gas turbines that power an air-separation unit (oxy-firing in a refinery), the addition of these GHGs did not have a significant effect on the life-cycle well-to-tank GHG emission results reported last quarter.

The project team continued to work investigators from the other subtasks to gather data on upgrading and is discussing how to quickly integrate ASPEN/PROMAX process model results from Subtask 6.1 with a life-cycle GHG estimation tool. Team members also contributed a section on carbon management to Subtask 6.3.

Subtask 3.2 - Flameless Oxy-gas Process Heaters for Efficient CO_2 Capture

During this quarter, the project team attempted multiple simulations of the OXYFLAM experiments conducted by the International Flame Research Foundation (IFRF) in 1995-1996 in the IFRF Furnace No. 2 (Lallement et al., 1997). In these tests, coaxial jets of fuel and oxygen were fired into a furnace with a cross section of 1.2 m x 1.2 m and a total length of 3.9 m. These tests were somewhat unusual in the regime of oxy-gas firing in that there was no flue gas recirculation (FGR), leading to high temperatures and potentially steep temperature and concentration gradients in the near-burner region. Multiple simulations of the near-burner region were attempted for a variety of oxygen and natural gas inlet velocities and for various heat loss conditions at the boundary, which were all parameters in the simulation test matrix defined in the previous quarterly report. Most simulations crashed within a few hours of startup. The few that ran long enough to restart crashed shortly after restarting. The reaction chemistry table was evaluated for possible problems, but none were found. It is like that the steep gradients produced by the firing configuration are causing numerical instability.

Project team members attended an IFRF conference in Glasgow, Scotland in June and learned of a recent oxy-gas experimental dataset featuring a new burner, the ENEL TEA-C burner, and the option for flue gas recirculation (Coraggio and Laiola, 2009). In these experiments, the recycled flue gas is first mixed with O_2 prior to combustion with the natural gas. Measurement taken in these flames include temperature and species concentration of O_2, CO_2, NO_x, and CO. The project team has decided to focus simulation efforts on this new dataset.

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

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

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

During this quarter, the project progress has included further modification to the geometry and mesh generation and the performance of a simulation with simple geometry in order to obtain initial understanding of all involved processes.

First, complications with Gambit, including demanding memory loads and body-uniting failures, have led to an unsuccessful geometry creation. Significant amounts of time were spent to solve this problem and to find an alternative direction to move this project forward, including consultations with CD-Adapco, the company behind Star-CCM+. Star-CCM+ has demonstrated the ability to handle large (on the order of a thousand bodies) geometry operations and has been selected for geometry handling in place of Gambit. EDEM simulations are still used to create randomly-spaced pieces of shale and to provide geometry data, which are now directly post-processed in Matlab to create a java script to be used with Star-CCM+. This java script is then used in Star-CCM+ to create all specified pieces of shale and unite them into a solid region. In comparison to Gambit, initial tests using Star-CCM+ have shown success in decreasing the time to create the geometry and in increasing the uniting operations capability, both requirements for creating a geometry with such a large number of particles. Figure 1 shows an image of a 1000+ body geometry united in Star-CCM+.

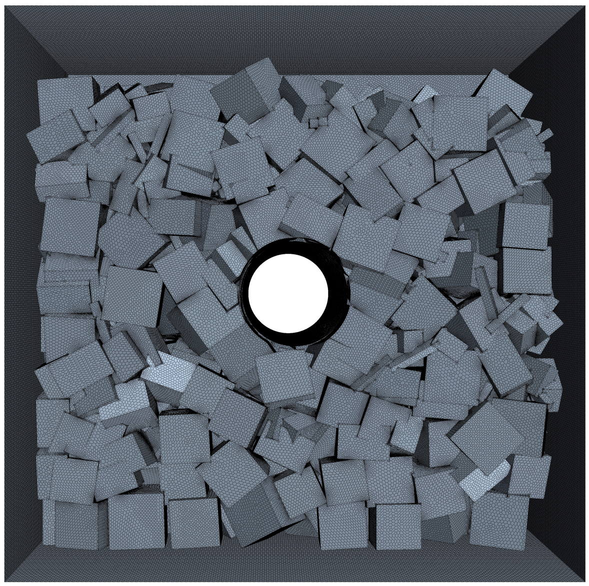

Figure 1: Complex shale geometry created in Star-CCM+.

Second, in order to create a computational fluid dynamics (CFD) simulation tool for use in validation studies of the Red Leaf ECOSHALE capsule, computational efforts are divided into three main tasks: 1) to correctly model heat transfer in the fluid region of the computational domain, including flow around obstacles, 2) to correctly model heat transfer inside the solid regions, and 3) to couple physics for both the fluid and solid regions into one simulation. The project team's current efforts are focused on task 1, e.g. obtaining accurate heat transfer in the fluid region, both empty and with obstacles. The initial simulation of pipe heating with no solid objects was two-dimensional and unsteady. A Reynolds-Averaged Navier-Stokes turbulence model was used. The test geometry, along with the developing velocity field, is shown in Figure 2. The temperature distribution for the same simulation is shown in Figure 3. As both velocity and temperature results for the 2-D case were satisfactory and as expected, the simulation was extended to a three-dimensional space with similar results.

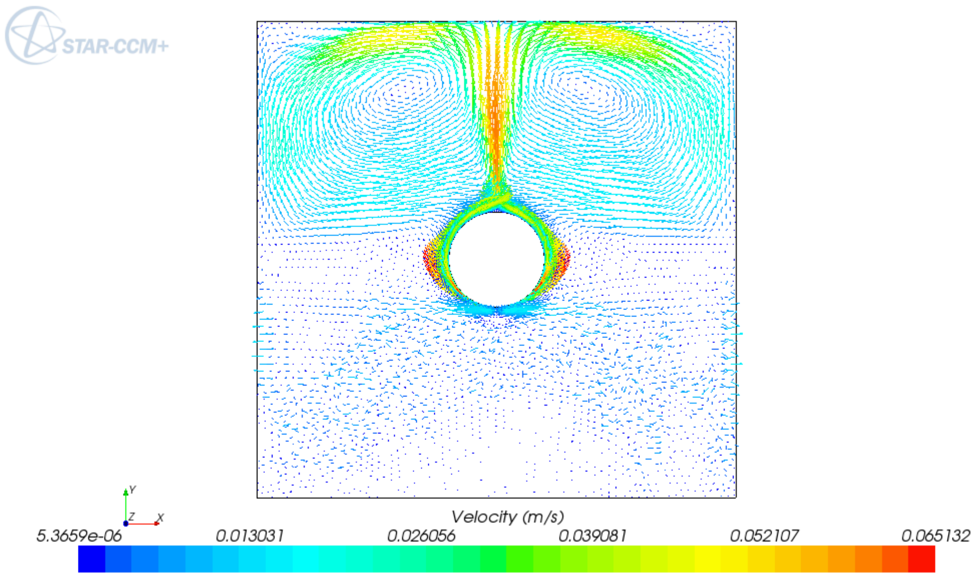

Figure 2: Velocity field for the initial 2-D RANS simulation.

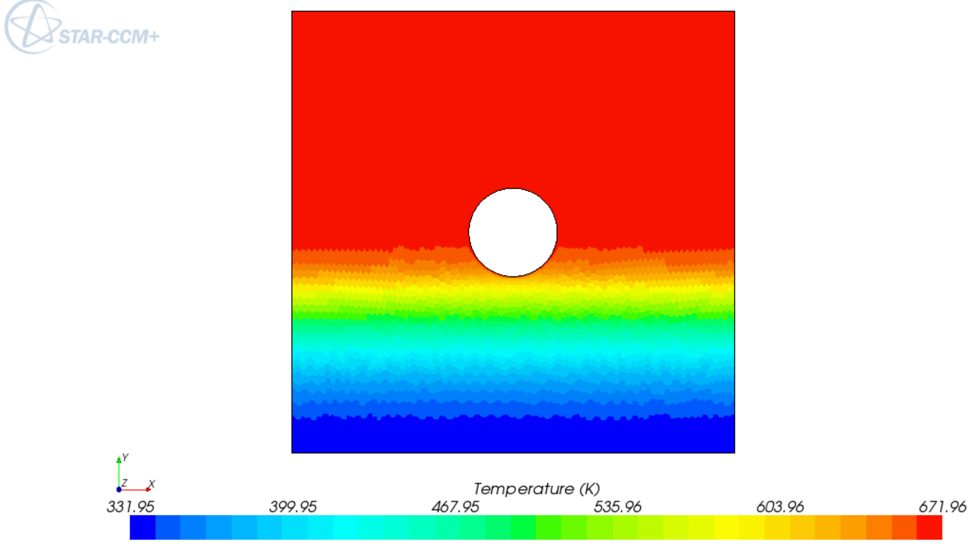

Figure 3: Temperature distribution for the initial 2-D RANS simulation.

Next, the project team introduced solid objects generated by EDEM into the domain, shown in Figure 4, and changed from RANS to Large Eddy Simulation (LES) turbulence models. LES models are able to resolve the unsteady vortex structures created by convective heat transfer in the domain, providing a more realistic simulation in comparison with RANS models. However, the preliminary results from this simulation do not show the proper heat transfer within the computational domain. As shown in Figure 5, the maximum temperature in the domain is around 820 K, much larger than the temperature of the heated pipe, which is 674 K. This error is attributed to insufficient mesh quality in the computational domain.

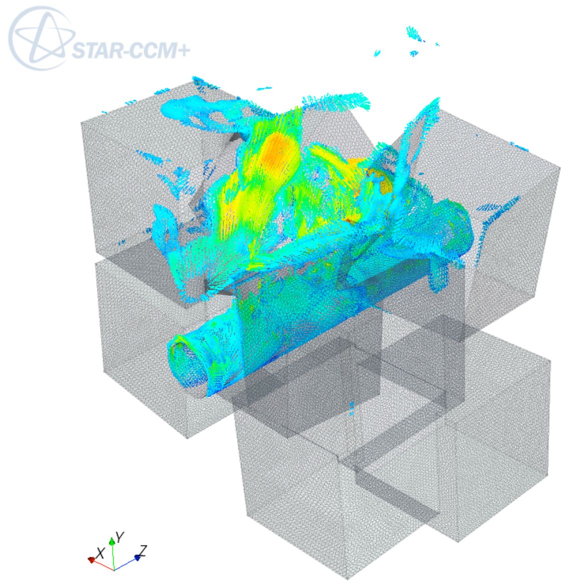

Figure 4: Initial 3-D LES simulation with obstacles. Also shown are velocity vectors for the preliminary simulation.

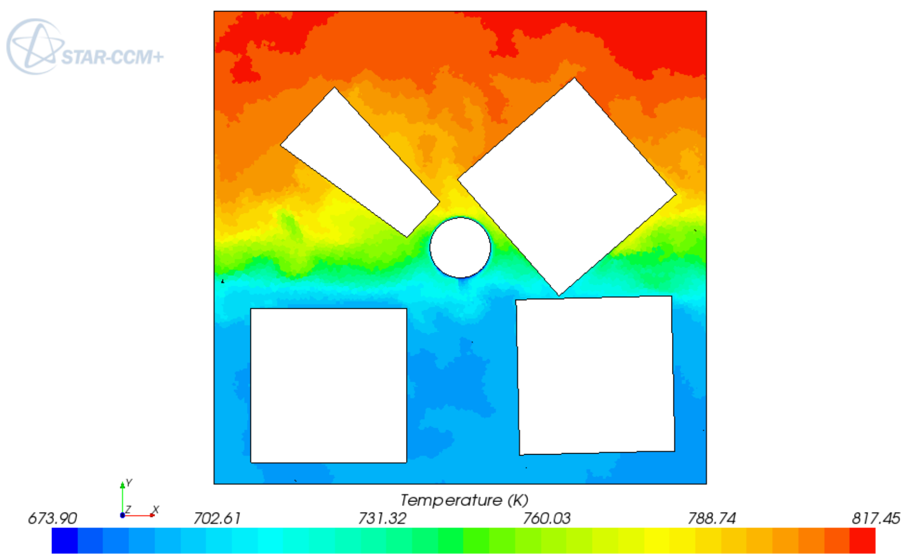

Figure 5: Temperature contours from the preliminary 3-D LES simulation.

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

As noted in the previous quarterly report, discussion among researchers in Task 4.0 has focused on obtaining a fresh core sample from the Mahogany zone of the Green River Formation in Utah's Uinta Basin. An opportunity arose this quarter to obtain such a sample by piggybacking on the spring drilling program of Oil Shale Exploration Company (OSEC).

ICSE and the Utah Geological Survey (UGS) teamed up to drill 1000 feet of 4-inch diameter core in the upper Green River Formation oil shale deposits in the eastern Uinta Basin, Utah, in May 2010. The purpose was to recover nearly the entire oil shale zone (Parachute Creek Member), providing “fresh” samples for a variety of geochemical and geomechanical tests. The coring team was led by Gary Aho from Sage Geotech and Michael Vanden Berg from the Utah Geological Survey (UGS). The well, Skyline 16, was located in Uintah County, Utah, T11S, R25E, Sec. 9, UTM E 661444, UTM N 4415107 (NAD83).

The well was spudded on May 18, 2010 in the upper Green River Formation, very near the Uinta/Green River Formation contact (in fact, the boundary could be seen on the hill side next to the drill rig). Over the course of seven days, the project team recovered 986 feet of continuous core, starting at 20 feet below surface down to a total depth of 1006 feet. Since oil shale is a very competent rock and cores very well, the drillers were able to use a 20-foot whole core barrel for the majority of the drilling, saving significant time. The drill rig is shown in Figure 6 while a section of the core immediately after recovery from the core barrel is shown in Figure 7. The drilling occurred as follows:

- May 18, 2010 – Cored 20.0 to 41.8 ft (total ~22 ft) – Rotary drilled, cemented, and cased from surface to 41.8 ft, needed to let cement cure over night
- May 19, 2010 – Cored 41.8 to 212.0 ft (total ~170 ft) – The vuggy Birds Nest interval was cored with the 10-foot split barrel to achieve better recovery
- May 20, 2010 – Cored 212.0 to 412.6 ft (total ~200 ft)
- May 25, 2010 – Cored 412.6 to 564.3 ft (total ~150 ft) – Late start, drillers drove from Grand Junction, CO in morning after four days off
- May 26, 2010 – Cored 564.3 to 745.4 ft (total ~180 ft)
- May 27, 2010 – Cored 745.4 to 905.9 ft (total ~160 ft) – Drilling slowed due to depth, replaced frayed winch cable (2 hour delay)
- May 28, 2010 – Cored 905.9 to 1006.3 ft (total ~100 ft) – Logged well after drilling was completed

Figure 6: Drill rig in the eastern Uinta Basin.

Figure 7: Section of 4-inch core.

During drilling, special care was taken to preserve the core for future testing. Starting at 260 feet and continuing down to about 700 feet, the core was slid into thick plastic sleeves and sealed with duct tape to help preserve the core's moisture. In addition, 12 1-foot sections (1 from the A-groove, 8 from the Mahogany Zone, 1 from the B-groove, and 2 from the upper R-6) of core were wrapped in plastic wrap and sealed in ProtecCore, a special aluminum sleeve designed to preserve core in an in-situ state. The core was trucked to Salt Lake City and is stored at the UGS Core Research Center. In the next few months, the core will be slabbed with a 1/3rd-2/3rd cut; the 1/3rd slab will be placed in display boxes and archived for future research and viewing, while the 2/3rd section will be placed back in the protective sleeves and reserved for future sampling/testing.

Figure 8 displays the stratigraphy of the core including geophysical logs, a preliminary designation of lithologic units (rich and lean zones), and a preliminary core log showing location of sand and tuff beds. A much more detailed core log will be constructed in the coming months.

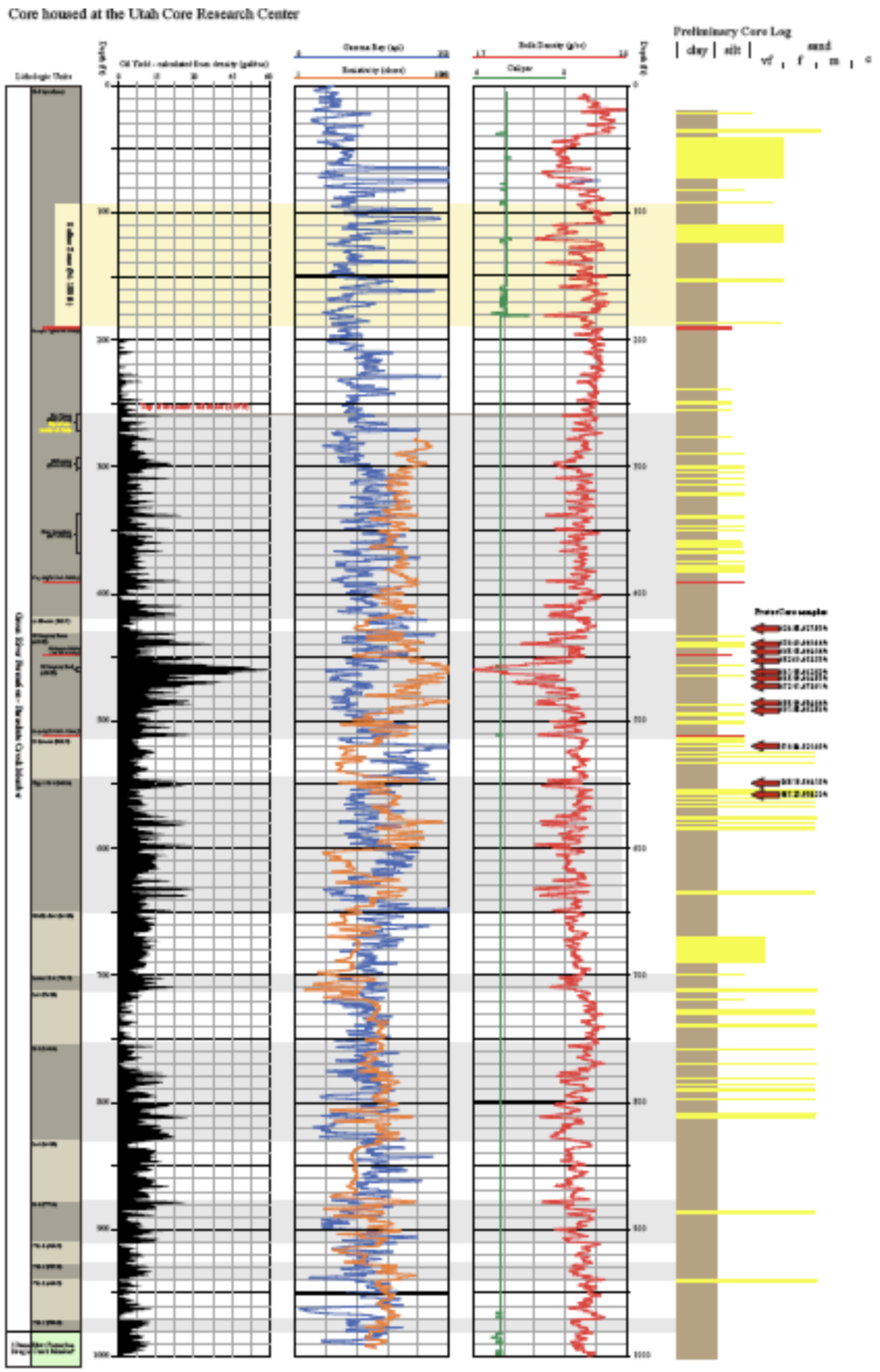

Figure 8: Stratigraphy of the core.

The project team also performed work relative to in-situ production models. Calculating multiphysical phenomena with a wide range of time scales is a significant challenge for in-situ oil shale dynamics modeling. Chemical kinetics, heat transfer through reservoirs by conduction and convection, phase changes, geomechanics, and multiphase flow are the physical processes involved. An appropriate balance between computational cost and accurate physical representation is important. Experimental design techniques have been used to understand the interplay and significance of various physical parameters. Fractional factorial experimental designs were used to expose the parameters of greatest importance in calculated results. The parameters studied were chosen based on judgment and interest. STARS, a commercial simulator capable of calculating reactive thermal reservoir processes, was used in these studies.

The reaction mechanism used by the researchers consists of a series of reactions representing seven pseudo components.

Reaction 1	Kerogen -> HO + LO + gas + CH_4 + char
Reaction 2	HO -> LO + gas + CH_4 + char
Reaction 3	LO -> gas + CH_4 + char
Reaction 4	Gas -> CH_4 + char
Reaction 5	Char -> CH_4 + gas + coke

The parameters chosen were: (1) Molecular weight of kerogen/stoichiometry/initial kerogen molar concentration (these values are treated as one parameter since they are dependent on each other to conserve volume and mass balances), (2)-(5) activation energies for reactions 1-4, (6) with/without normal distribution of activation energies for reaction 1, (7) relative permeability representation, and (8) reaction enthalpy. The parameters that had the greatest impact on the ultimate recovery of oil at the scale of study were activation energy for Reaction 1, activation energy for Reaction 3, a distribution of activation energies for Reaction 1, relative permeability representation, and the interactions between these parameters. These four significant parameters were explored further with a full factorial experimental design to create a response surface model with the following form:

$$y = \beta_o + \sum_{i=1}^{k} \beta_i x_i + \sum_{i \neq j}^{k} \sum \beta_{ij} x_i x_j + \sum \sum \sum_{i \neq j \neq l} \beta_{ijk} x_i x_k x_l + \beta_{ijlm} x_i x_j x_l x_m$$

Monte Carlo simulations were run to characterize this response surface and to provide a method for uncertainty quantification where the variation in the significant input parameters affect the distribution of the output (ultimate recovery of oil). A few random validation runs were simulated to compare the response surface results to simulated results. The accuracy of the response surface ranged from 3% to 15% error for predicting full simulations. This accuracy could be improved by reducing the size of the experimental space, or by running additional simulations to estimate curvature due to nonlinearities.

Geomechanics may also play a significant role in the ultimate recovery of oil as it influences the relationship between porosity (created as solid kerogen is converted to fluids) and permeability (the expelling of fluid from pore space). Fluids can also convert to residual solids at the high temperatures involved, which could plug permeable pathways. An exponential relationship between porosity and permeability can be used in STARS.

$$k = k_o \cdot \exp\left[k_{mul} \cdot \left(\frac{\varphi - \varphi_o}{1 - \varphi_o}\right)\right]$$

Here k_o and φ_o are the initial fluid porosity and permeability and k_{mul} is an empirical multiplier. The sensitivity of simulated results to this multiplier has been explored. Figure 9 shows preliminary results where the oil composition was affected by the multiplier. Further studies will explore the significance and interactions of this multiplier together with the other physical parameters discussed.

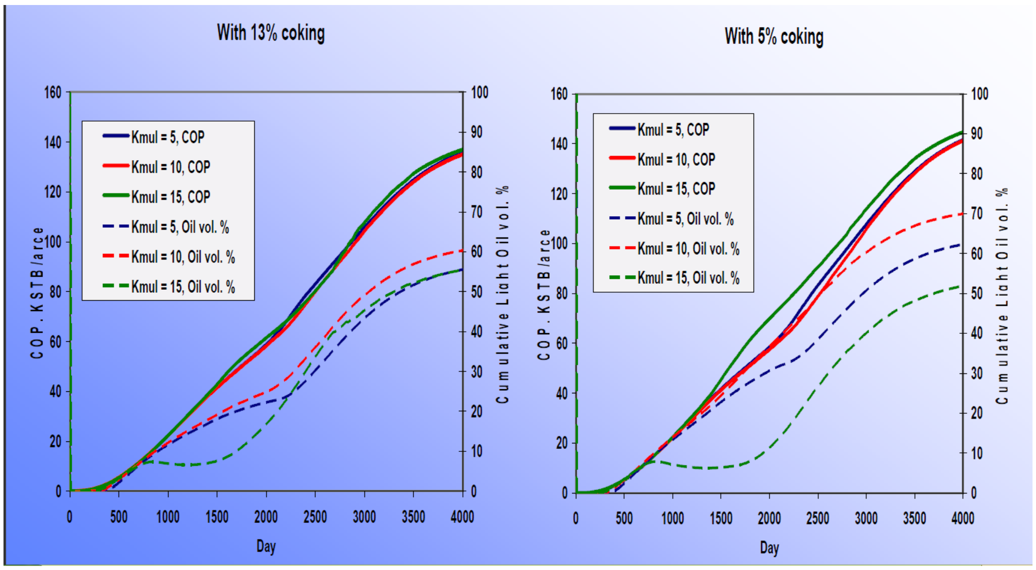

Figure 9: Preliminary results showing how cumulative oil production (COP) is affected by the permeability multiplier with different amounts of assumed coking.

Subtask 4.3 – Multiscale Thermal Processing of Oil Shale

In this quarter, the kinetic parameters of thermal decomposition (pyrolysis) of fine powdered Green River oil shale samples in thermal gravimetric analyzer (TGA) experiments were calculated using different kinetic models (Table 1). This collection of models is suitable for studying complex materials. The Kinetic05 model package, developed at Lawrence Livermore National Laboratory, was used for the analysis.

Table 1. Kinetic parameters generated from different models.

Kinetic models		*E (kJ/mol)*	*A (1/s)*	*Order*	*Paremeter-1*	*Paremeter-2*
Gaussian	n = n	180.061	8.12E+10	0.53	4.19E+00	
	n = 1	181.446	1.29E+11	1.00	3.78E+00	
Discrete	Case-1	Fig 7-(a)	5.72E+09	1.00		
	Case-2	Fig7-(b)	1.00E+14	1.00		
	Case-3	Fig7-(c)	$e^{(a+bE)}$	1.00		
Weibull		163.154	6.64E+09	1.00	1.04E+04	9.99E+00
1st order		156.968	2.19E+09	1.00		
nth order		160.735	5.80E+09	1.65	1.65	
Isoconversional		Figure-8		1	Friedman based	

The results were compared with parameters from model-free advanced isocoversion models, which were described in earlier reports. The distributions of kinetic parameters were obtained and kinetic model reconstructions were set up for different models. Figure 10 shows experimental and model comparisons for a heating rate of 10°C/min. The goodness of fit (root mean square errors) for the different kinetics models are compared in Figure 11. Isoconversional models appear best suited to describe the data. These methods capture the complex chemistry involved in the solid decomposition and reflect the shift in the controlling mechanism step in terms of distributed kinetic parameters. The kinetic parameters obtained from the model free isoconversion method (Isokin) were used to extrapolate the pyrolysis conditions to real field applications, e.g. in-situ pyrolysis and flash pyrolysis; see Figure 12.

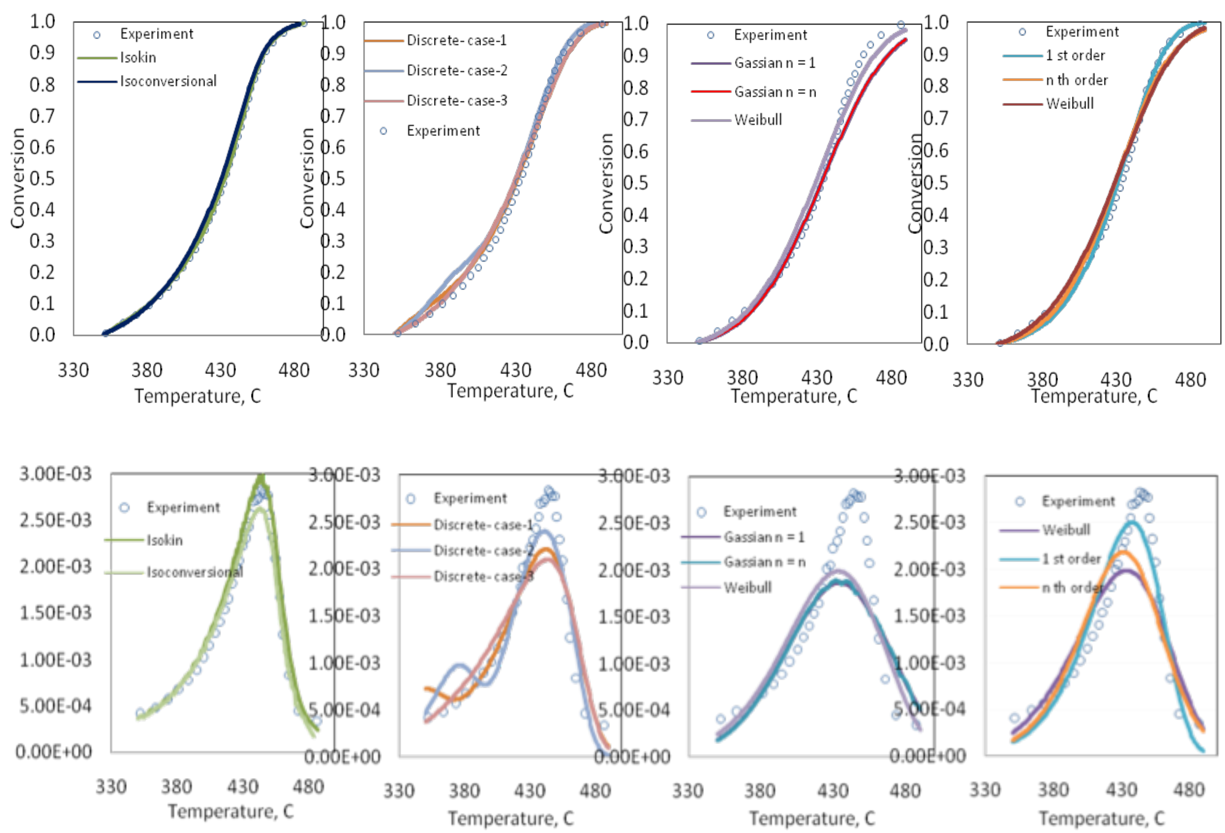

Figure 10: Comparison of the kinetic models (top - conversion, bottom - rate).

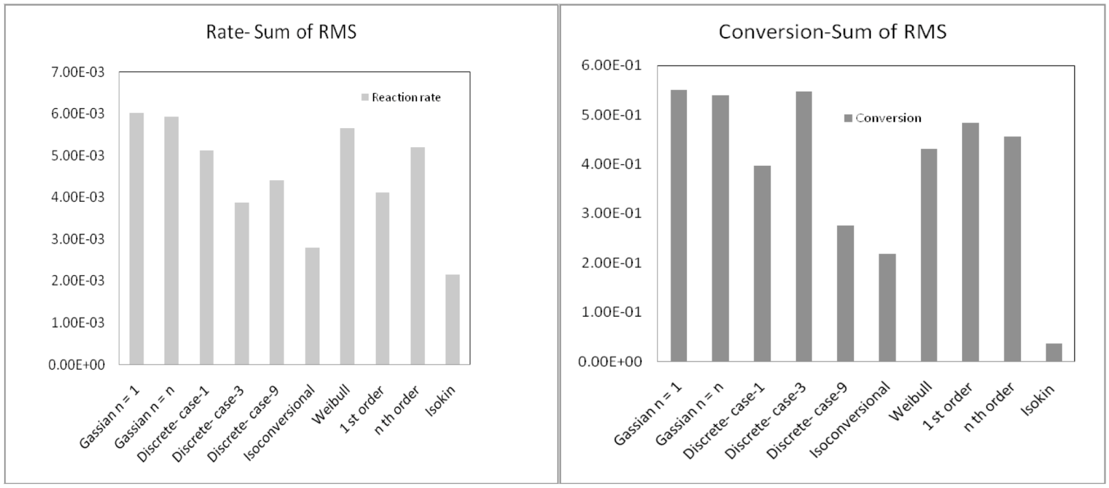

Figure 11: Comparison of the kinetic models based on sum of RMS of residues.

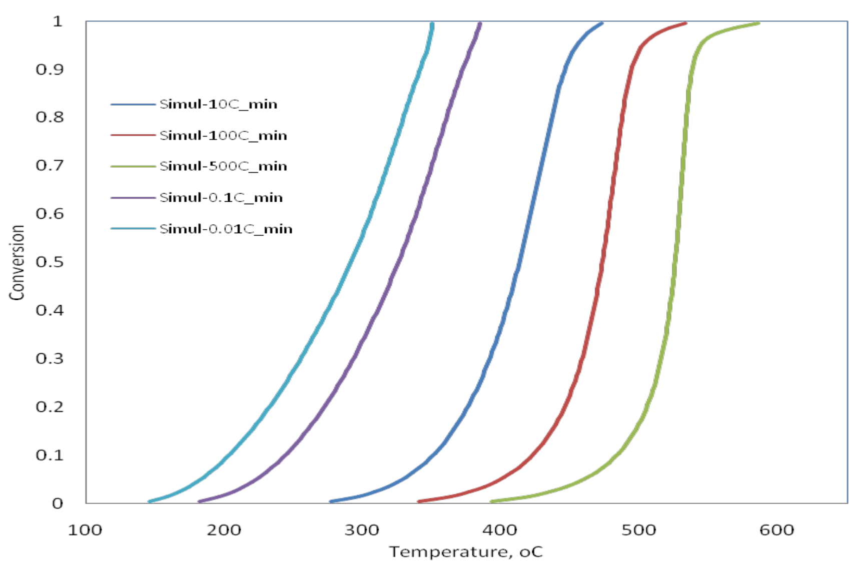

Figure 12: Simulated conversion profiles at extrapolated constant heating rates.

Subtask 4.4 - Effect of Oil Shale Processing on Water Compositions

In the previous quarterly report, the apparatus to perform hydrous and anhydrous pyrolysis experiments was described. In this quarter, the project team completed six hydrous experiments at various conditions. The pressure increases during each of the experiments were recorded. Water and oil samples were collected. The water samples will be sent out for analyses to measure organic concentrations. Team members in discussion with a local vendor (DataChem) about the types of analyses and the compounds to be measured.

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

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

During this quarter, 3 drill cores, each 15 cm long, were pyrolyzed at different reaction temperatures in the pyrolysis reactor. The core was heated from the outside using a band heater. A heating rate of 100°C/min was used to get to the reaction temperature, where the core was held for 24 hours. Nitrogen was flowed at a steady rate of 55 ml/min during the experiment. The condensate was collected in a series of two condensers held at -6°C. The core was cooled to ambient temperature, removed from the reactor, and subjected to X-ray microtomography (XMT) analysis as described below. The pyrolysis conditions are summarized in Table 2.

Table 2. Sample number of oil shale pyrolysis at three different reaction temperatures.

Sample No.	Type	Temperature (°C)	Mode
MD-3	¾" drill core	300	N_2 flow
MD-4	¾" drill core	350	N_2 flow
MD-5	¾" drill core	400	N_2 flow

The project team then obtained the pore network structure that evolved during pyrolysis at different temperatures through image digitalization. Figure 13 shows the 3-D volume rendered images from the reconstructed XMT data (~5 micron voxel resolution) for the Mahogany oil shale drill core samples after pyrolysis at reaction temperatures of 300°C, 350°C, and 400°C, respectively. Some of the pore space created during pyrolysis is clearly visible at this resolution and it is possible to distinguish between the pyrolyzed oil shale and the host shale rock. Crack networks, developed during the pyrolysis process, are evident and well defined. Two distinct regions with different sizes of cracks and voids are identified. As indicated from our previous report, cracks and voids as small as 100 nm (from X-ray nanotomography, XNT, images) were observed inside the silicate-rich lamellar structure. However, larger, anisotropic cracks and voids have developed inside the kerogen-rich lamella structure as shown from high resolution X-ray microtomography (HRXMT) images presented in Figure 14.

The crack networks and voids inside the kerogen-rich lamellar structure of the pyrolyzed oil shale samples are highly anisotropic. In this regard, the absolute permeability is determined based on the coupling of Lattice Boltzmann (LB) simulation with HRXMT subset data obtained from kerogen-rich regions containing more cracks (e.g. the deduced pore structure). Figure ** shows the 3-D views of LB simulated flow along the x-axis through the reconstructed HRXMT image of oil shale pyrolysis products at the three reaction temperatures. Once the solid phases are removed, the right-hand side of Figure 14 shows the nature of the flow channels. The velocity scale is color-coded as shown by the color bar in the figure. Solids are white and solution velocity ranges from black for no flow, through blue, green, yellow and finally red for the highest flow rate. Table 3 summarizes the estimated permeability for the bedding plane of the kerogen-rich layer from the pyrolyzed oil shale samples.

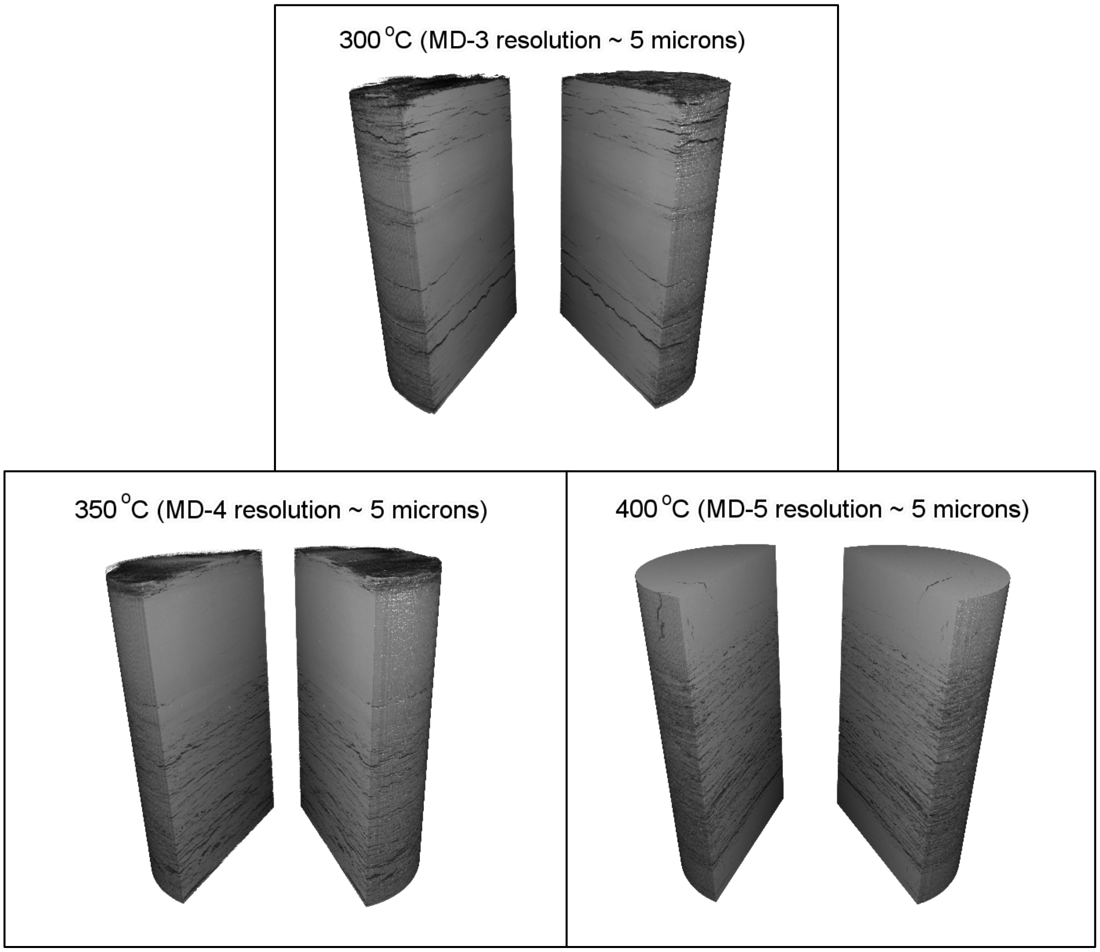

Figure 13: Volume rendered images of Mahogany oil shale drill core samples after pyrolysis at reaction temperatures of 300˚C (MD-3), 350˚C (MD-4), and 400˚C (MD-5) from reconstructions of HRXMT data at ~5 µm voxel resolution. Gray scale level indicates variations in the X-ray attenuation coefficients, which depend on density and atomic number of material within each voxel. Light regions are the silicate-rich lamella layers, dark regions are kerogen-rich lamella layers.

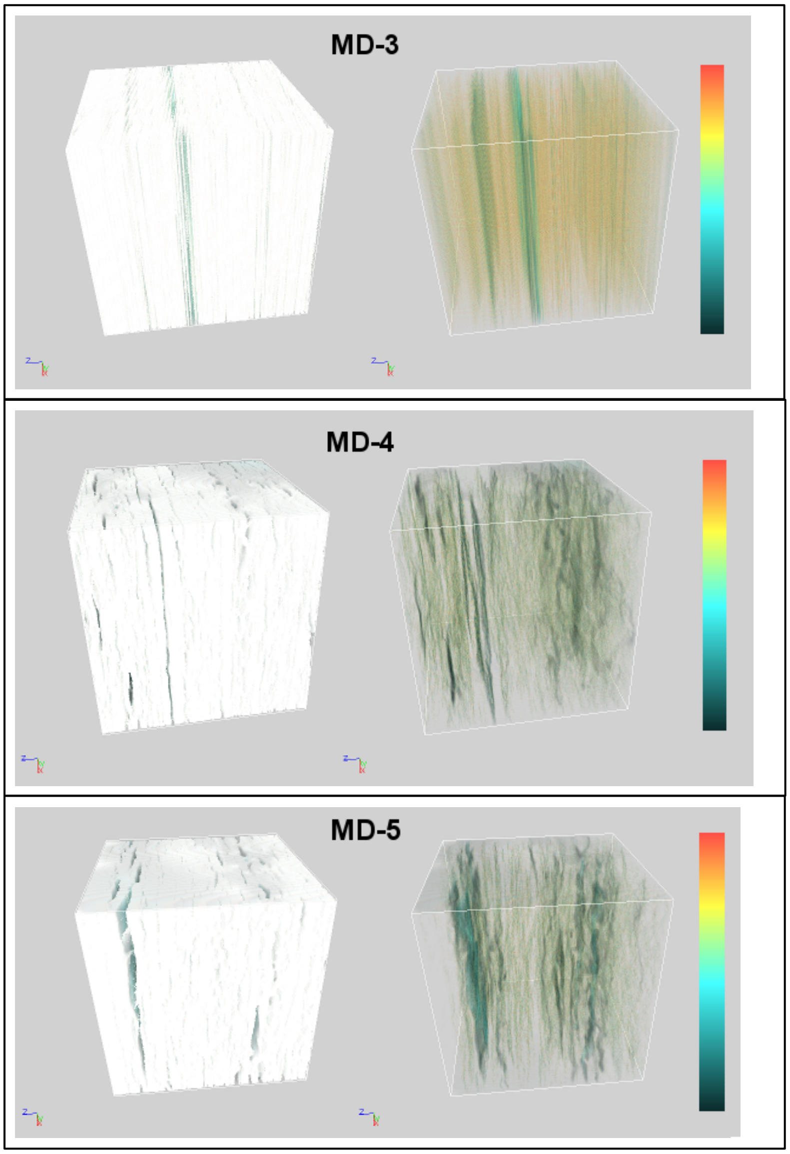

Figure 14: 3D views of LB simulated flow along x-axis (direction of the bedding plane) through reconstructed HRXMT image of kerogene-rich region for oil shale pyrolysis products at different reaction temperatures (300˚C - MD-3, 350˚C - MD-4, and 400˚C - MD-5); solid phase is transparent to reveal flow channels.

Table 3. Estimated permeability for kerogen-rich region of pyrolyzed oil shale samples at different reaction temperatures.

Sample No.	Temperature (^oC)	Mode	Estimated Permeability (darcy)
MD-3	300	N_2 flow	6.77
MD-4	350	N_2 flow	3.23
MD-5	400	N_2 flow	3.87

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

In this quarter, the project team switched from kerogen modeling to modeling of the asphaltene structures present in oil sands. This work mirrors that previously done on the kerogen model.

The work has focused on the set of six 2-D representative asphaltene structures reported by Siskin et al. (2006). These structures were established based on experimental data measured on asphaltene samples from six different locations around the world. The project team first built 3-D modules using HyperChem and molecular mechanic level calculations then used ab initio calculations (GAMESS, RHF with STO-3G basis sets) to further optimize these structures. Attention was paid to the flexible bridging groups present in all of the asphaltene structures as changes in this portion of the structure greatly affected the energy (stability) of the system.

Additionally, it has been reported that these asphaltene units tend to stack as a result of intermolecular forces between the units. The preferred stacking orientation was studied on one of the asphaltenes (Campana model). The calculations to look at the stacking were first done at the Density Functional Theory (DFT) level using the new M06-2X functional that was developed for the study of non-bonding interactions using stacks of three Campana units. Three different stacking patterns (parallel or stacked one above each other, anti-parallel or stacked above each other but also rotated 180° about the major plane of the asphaltene, and inverted or stacked above each other and also rotated 180° about the other axis of the unit) were studied, and the parallel stack was found to be the lowest in energy; this makes sense at it is the orientation that allows for the closest stacking. Calculations are now proceeding at the molecular mechanic level of theory on stacks of 20 units.

Finally, work also began on modeling of inorganic matter in order to study interactions between the organic kerogen/asphaltene models and the inorganic material. Team members now have a 3-D structure of illite (an aluminum silicate clay structure) ready to use in these studies.

The project team is still holding the manuscript from last year entitled “Three-Dimensional Structure of the Siskin Green River Oil Shale Kerogen Model: A Computational Study” until team members can get atomic pairwise distribution function (PDF) from small angle X-ray scattering data on a kerogen sample taken from the core sample that ICSE obtained at the end of this quarter. This experimental data will be used to evaluate the 3-D kerogen model obtained by computational efforts in this task.

Task 5.0 - Environmental, Legal, Economic and Policy Framework

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

During this quarter, Subtask 5.1 research focused primarily on issues related to wildlife and plants and on access to oil shale and oil sands resources. With respect to wildlife and plants, the project team researched international law regarding migratory bird protection, recent litigation resulting from inadequate tailings pond management in Alberta, and the litigation’s precedential value for prospective U.S. oil shale or oil sands operators. Research also looked at designated wild horse and burro management areas within the Uinta Basin, applicable management requirements, and their potential impact on oil shale or oil sands development. Subtask 5.1 researchers also reviewed (and will continue to monitor) draft federal legislation regarding wildlife migration corridors and evaluated the most recent Endangered Species Act listing of plants found on portions of the Mahogany Outcrop within Colorado and the likely impacts of those listings on oil shale development. With respect to resource access, research focused on (1) newly enacted Utah statutes promoting condemnation of federal lands to improve access to state lands surrounded by federal lands, (2) proposed federal legislation intended to force sale of certain federal lands, including BLM-managed lands within the Uinta Basin, and (3) implementation of the recently enacted Utah Recreational Land Exchange Act, which transfers certain oil shale-bearing lands to the State of Utah. Members of the project team also attended a conference on the past, present and future of federal public land management that was hosted by the University of Colorado.

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

During this quarter, Subtask 5.2 research focused on issues associated with water resources and produced water, including analysis of historic water law insofar as it relates to water rights that vested prior to enactment of the current Utah water code. The project team identified and reviewed scholarly publications regarding integrated water resource management, beneficial use of water produced during natural gas extraction, and disposal requirements applicable to water produced during natural gas extraction. Research also focused on Wyoming statutory and case law regarding water produced during natural gas extraction as well as formal Attorney General opinions regarding produced water appropriation and management. Team members continue to monitor pending federal legislation regarding hydraulic fracturing as potentially relevant to oil shale and oil sands development. Members of the project team also attended a conference on energy resources and produced water, hosted by the University of Wyoming, that addressed water quality, water management, effluent treatment and produced water use.

6.0 – Economic and Policy Assessment of Domestic Unconventional Fuels Industry

Subtask 6.1 Engineering Process Models for Economic Impact Analysis

Progress has been made during the quarter on delivering a draft report for one scenario, e.g. the underground mining, surface retorting, upgrading and transportation oil from Uinta Basin oil shale. This deliverable was delayed slightly from its due date. The work on the other scenarios, in-situ and ex-situ extraction of oil sands, in-situ extraction of oil shale, and in-situ extraction of heavy oil from the North Slope of Alaska, has been progressing nicely. The model building is now done due to the over time efforts of the project team with the exception of the in-situ oil shale extraction scenario. Included as a supplement to this quarterly report is an Excel file that is the deliverable required for Subtask 6.1 for this quarter. The file includes (1) upstream supply costs and listing of materials and (2) equipment and services needed for facility construction and for on-going operations and maintenance for each scenario. Some of the results of the economic analysis are remarkable in that the royalty and tax rates play a very large role in the supply costs, often more so than any other cost category. Multiple runs of the project team's mass and energy balance software were required for the upgrading of each fuel to provide the details needed for supply cost calculations. These mass and energy balance simulations for all the scenarios are performed off-line and uploaded to Excel for the supply cost calculations. Various sensitivity analyses are easily performed with this Excel file and graphically presented as bar charts of the various contributors to the cost per barrel of synthetic crude oil produced. With this work complete, the project team can now perform sensitivity analysis and begin writing for Subtask 6.3, the Market Assessment report.

Also in this quarter, the project team travel to Rifle, CO, for a presentation and meeting with Sage Geotech, a consulting group for the oil shale industry. Sage provided invaluable input and data for the development of the oil shale scenarios and assessed the accuracy of the project team's results.

Subtask 6.2 - Policy analysis of the Canadian oil sands experience

The project team focused on researching and preliminary drafting of report sections addressing differences between the United States and Canada in terms of taxes and royalties levied on oil sands production as well as downstream and marketing challenges facing oil sands development. Drafts of these two sections are included in Appendix C. Progress on these sections was delayed somewhat due to the unexpected premature delivery and subsequent maternity leave of one member of the project team. However, this delay is not expected to significantly impact the overall progress or timeliness of Subtask 6.2 beyond this quarter. Research conducted this quarter included reviewing economic studies examining the effectiveness of varying tax and royalty regimes on oil sands investment and production, as well as conducting comparative analyses of U.S. and Canadian taxation and royalty configurations. The project team also focused on downstream demand challenges associated with refined products (e.g. jet and diesel fuel and heavier residuals) and anticipated supply issues relevant to oil sands development (e.g. current projects and plans in place to increase supply of oil sands crude in the U.S. to reach the complex refineries in the Gulf Coast area and to convey oil sands crude to other foreign markets, particularly Asia). Team members have also begun to look at the impacts of the British Petroleum Gulf Coast oil spill on the public perception of, and evaluation of environmental externalities associated with, oil sands production.

Subtask 6.3 – Market Assessment Report

The project team has focused this quarter on completing the various elements that will make up the Market Assessment report. One of those elements, an assessment of impacts to revenue corresponding to each scenario defined in Subtask 6.1, is largely complete. A draft of this assessment is included in Appendix D.

To complete this assessment of impacts to revenue, the project team gathered data and created models for implementing the chosen methodology to carry out a sensitivity analysis on the monthly revenue for each scenario. Team members gathered two categories of data: price forecasts created by the Energy Information Administration (EIA) and oil price and cost index data for the purpose of calibrating the oil price models. The price forecasts are of oil, natural gas, and electricity prices (a mix of regional and national-level forecasts) generated by the EIA's NEMS model and published in the Annual Energy Review. The oil price data is the monthly "refiner's domestic acquisition price" since 1974, and the producer's price index, also monthly since 1974. Only minor preliminary work on the data was necessary (e.g. converting units of measurement).

Team members chose price models that are commonly used for similar purposes. Data on oil prices (deflated by the Producer Price Index) was used to estimate the parameters of these models. For each model, the output is the probability distribution of price implied by that model at each point in time for a time horizon of 20 years. A discretized version of each model can also be used to simulate any number of price paths. An Excel add-in will be used to carry out the simulations of these price paths in the project team's financial spreadsheet, yielding probability distributions for measures of profitability (e.g. the internal rate of return and net present value).

CONCLUSIONS

The Clean and Secure Energy from Domestic Oil Shale and Oil Sands Resources program hosted the University of Utah Unconventional Fuels Conference on April 28, 2010. Conference attendees exceeded 130. The speech by Steve Black, Counsel to Secretary of Interior Salazar, generated much media interest. Research work continued in the four main thrust areas of the program. In the area of oil shale and sands utilization with CO_2 management, the project team is working with investigators from Subtask 6.1 to quickly integrate ASPEN/PROMAX process model results with a life-cycle GHG estimation tool. In the area of liquid fuel production from in-situ thermal treatment of oil shale/sands, the research team obtained fresh, 4-inch diameter oil shale core from the eastern Uinta Basin of Utah by piggy backing on the OSEC spring drilling program. The coring project recovered nearly the entire oil shale zone (Parachute Creek Member). Additional research focused on continued development of geologic, kinetic, porosity, and atomistic models that can be applied to a reservoir-scale process. In the area of environment and policy, research work focused on issues related to wildlife and plants, on access to oil shale and oil sands resources, and on issues associated with water resources and produced water, including analysis of historic water law insofar as it relates to water rights that vested prior to enactment of the current Utah water code . In the market assessment area, a spreadsheet was developed that includes upstream supply costs and listing of materials plus equipment and services needed for facility construction and for on-going operations and maintenance for each unconventional fuels development scenario. Additionally, draft versions of report sections addressing (1) differences between the United States and Canada in terms of taxes and royalties levied on oil sands production (2) downstream and marketing challenges facing oil sands development, and (3) assessment of impacts to revenue corresponding to each unconventional fuels scenario were completed.

COST STATUS

Baseline Reporting Quarter	Yr. 1							
	Q1		Q2		Q3		Q4	
	7/1/09 - 12/31/09		1/1/10 - 3/31/10		4/1/10 - 6/30/10		7/1/10 - 9/30/10	
	Q5	**Total**	Q6	**Total**	Q7	**Total**	Q8	**Total**
Baseline Cost Plan								
Federal Share	484,728	**484,728**	484,728	**969,456**	484,728	**1,454,184**	484,726	**1,938,910**
Non-Federal Share	121,252	**121,252**	121,252	**242,504**	121,252	**363,756**	121,254	**485,010**
Total Planned	605,980	**605,980**	605,980	**1,211,960**	605,980	**1,817,940**	605,980	**2,423,920**
Actual Incurred Cost								
Federal Share	420,153	**420,153**	331,481	**751,634**	547,545	**1,299,179**		**1,299,179**
Non-Federal Share	29,456	**29,456**	131,875	**161,332**	151,972	**313,304**		**313,304**
Total Incurred Costs	449,609	**449,609**	463,356	**912,966**	699,517	**1,612,483**	0	**1,612,483**
Variance								
Federal Share	64,575	**64,575**	153,247	**217,822**	-62,817	**155,005**	0	**639,731**
Non-Federal Share	91,796	**91,796**	-10,623	**81,172**	-30,720	**50,452**	0	**171,706**
Total Variance	156,371	**156,371**	142,624	**298,994**	-93,537	**205,457**	0	**811,437**

Baseline Reporting Quarter	Yr. 2			
	Q5		Q6	
	10/1/10 - 12/31/10		1/1/11 - 3/31/11	
	Q8	**Total**	Q8	**Total**
Baseline Cost Plan				
Federal Share	323,403	**2,262,313**	323,402	**2,585,715**
Non-Federal Share	80,835	**565,845**	80,834	**646,679**
Total Planned	404,238	**2,828,158**	404,236	**3,232,394**
Actual Incurred Cost				
Federal Share		**1,299,179**		**1,299,179**
Non-Federal Share		**313,304**		**313,304**
Total Incurred Costs	0	**1,612,483**	0	**1,612,483**
Variance				
Federal Share	0	**963,134**	0	**1,286,536**
Non-Federal Share	0	**252,541**	0	**333,375**
Total Variance	0	**1,215,675**	0	**1,619,911**

MILESTONE STATUS

There were 15 milestones/deliverables scheduled for completion in this quarter. The milestones in Task 2.0, Technology Transfer and Outreach, were to hold both an industrial advisory board and project review (presentations/poster session at the ICSE-sponsored unconventional fuels conference) meetings, to implement Interactive Map usage tracking software, and to complete addition of research materials from each task/subtask in the Digital Repository. The first three milestones were completed as reported in the Task 2.0 summary above. The last milestone has been delayed due to the volume of documents that need to be uploaded. Materials for each task should be in the repository by the end of next quarter.

Subtask 4.1, the development of a CFD-based simulation tool for in-situ thermal processing of oil shale/sands, had a milestone to implement the correct geometry representation of the Red Leaf ECOSHALE capsule in Star-CCM+. While this task is not yet complete, significant progress was made in this quarter as reported in the Subtask 4.1 summary above. Subtask 4.2, the examination of in-situ production models, had a milestone to develop models with preliminary geomechanics & reactions. A model consisting of an exponential relationship between porosity and permeability was tested and results shown in the subtask summary above. In Subtask 4.3, the multiscale pyrolysis project, the two milestones were to complete mass balances for oil/gas/coke at different scales and to develop a preliminary kinetic model for oil shale pyrolysis. The project team has obtained the data and have been looking at it closely to determine how yields constrain the elemental information (C, H, N, etc). Hence, from the data point of view, the milestones have been accomplished. The analysis will be reported in the next quarterly report. The Subtask 4.4 milestone to complete preliminary analysis of process water, including some tables of aqueous phase organic species concentrations, has been delayed because the water samples obtained from pyrolysis experiments have yet to be sent out for analysis. Subtask 4.5, the pore-scale analysis project, had a milestone to perform XMT/XNT analysis of samples of pyrolysis products at different temperatures. This milestone was completed as reported in the subtask summary above.

For Subtask 6.1, engineering process models for economic impact analysis, the milestone was to deliver (1) upstream supply costs and a listing of materials and (2) equipment and services needed for facility construction and on-going operations and maintenance for each unconventional fuels scenario in the Market Assessment. This milestone has been completed with the summary provided above for Subtask 6.1 and the Excel spreadsheet included with this report. The Subtask 6.2 milestone was to prepare a preliminary report addressing differences between the U.S. and Canada in terms of taxes and royalties levied on production and in downstream/marketing challenges. This milestone has been completed and the draft report is included as Appendix C. Subtask 6.3 had three milestones. Significant progress was made during the quarter on the first milestone, to describe the methodology and preliminary results of a supply cost analysis for one scenario (underground mining and surface retorting of Uinta Basin oil shale), but the draft report was slightly delayed. A draft will be available before the end of the next quarter. The second milestone, to deliver an assessment of impacts to revenue corresponding to each scenario, has been completed and the draft report is included as Appendix D. The third milestone, a preliminary report summarizing the first three sections of the Market Assessment (role of unconventional fuels in current energy climate, role of policy & government, role of externalities & public perception) has been delayed by the work required to meet other milestones for assessment. It it anticipated that this delay will not affect the release of a draft Market Assessment report at the end of next quarter.

NOTEWORTHY ACCOMPLISHMENTS

For Task 4.0, the obtaining of a 4-inch fresh oil shale core from the eastern Uinta Basin of Utah is seen as a great opportunity to integrate research efforts across scales and to test the impact of fresh core on the results obtained from experiments at these scales.

PROBLEMS OR DELAYS

Due to visa problems, Dr. Lin will be unable to present his paper entitled "Pore scale analysis of oil shale pyrolysis by X-ray CT and LB simulation" at the September 2010 World Congress on Industrial Process Tomography in Beijing, China. The paper Dr. Lin was going to present has been submitted for inclusion in the conference proceedings.

For Task 2.0, the milestone to upload materials from each task/subtask to the Digital Repository was delayed due to the volume of documents. The Institute Librarian anticipates that materials for each task will be in the repository by the end of next quarter. For Subtask 4.1, team members were delayed in the completion of the milestone to implement the correct geometry representation of the Red Leaf ECOSHALE capsule in Star-CCM+ due to the need to take incremental steps in building capability. Recently, a post-doctoral fellow has joined the project team to help meet deliverables in a more timely manner. The Subtask 4.4 milestone to complete preliminary analysis of process water has been delayed by talks with DataChem, who will be performing the sample analysis. Team members expect analysis results next quarter. For Subtask 4.6, project team members are still holding the manuscript for "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 until they can get experimental atomic pairwise distribution function from small angle X-ray scattering data on a kerogen sample taken from the fresh 4-inch core sample that ICSE obtained this quarter.

While the Subtask 6.2 milestone to complete a draft report addressing differences between the U.S. and Canada in terms of taxes and royalties levied on production and in downstream/ marketing challenges was not delayed, the draft was not as complete as anticipated due to the unexpected premature delivery and subsequent maternity leave of one member of the project team. However, this delay is not expected to significantly impact the overall progress or timeliness of Subtask 6.2 beyond this quarter. The Subtask 6.3 milestone to prepare a preliminary report summarizing the first three sections of the Market Assessment was delayed due to project team members working on deliverables for the various subtasks that feed the assessment, including Subtasks 3.1, 6.1, and 6.2. This delay will not impact the release of a draft Market Assessment report at the end of next quarter.

RECENT AND UPCOMING PRESENTATIONS/PUBLICATIONS

Lauren P. Birgenheier and Michael D. Vanden Berg, "Integrated sedimentary and geochemical investigation of core form the upper Green River Formation lacustrine deposits, Uinta Basin, Utah." Poster presented at 2010 AAPG Annual Meeting, New Orleans, LA, April 12, 2010.

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

Jennifer Spinti, Philip J. Smith, and Brandon Hochstrasser, "Oxy-gas process heaters for efficient CO_2 capture." Poster presented at University of Utah Unconventional Fuels

Conference, Salt Lake City, UT, April 28, 2010.

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

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

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

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

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

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

I.S.O. Pimienta, A.M. Orendt, R.J. Pugmire, and J.C. Facelli, "3D structures of oil shale kerogen and tar sand asphaltenes." Poster presented at University of Utah Unconventional Fuels Conference, Salt Lake City, UT, April 28, 2010.

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

Benardo Castro, Milind Deo, Michael Hogue, Kerry Kelly, Terry Ring, Jennifer Spinti, Kirsten Uchitel, Jon Wilkey, "Unconventional fuels market assessment." Poster presented at University of Utah Unconventional Fuels Conference, Salt Lake City, UT, April 28, 2010.

C. L. Lin, A. R. Videla and J. D. Miller, "Advanced 3D multiphase flow simulation in porous media reconstructed from X-ray micro tomography using the He-Chen-Zhang Lattice Boltzmann model," *Flow Measurement and Instrumentation*, in press.

Jennifer P. Spinti, Jeremy N. Thornock, and Philip J. Smith, "Oxy-gas combustion for efficient CO_2 capture: Effect of near burner mixing on velocity and composition fields," Mixing XXII, Victoria, BC, Canada, June 20-25, 2010.

K. E. Kelly, A. F. Sarofim, and D. W. Pershing, "Opportunities for reducing CO_2 emissions from conventional and unconventional fuels using oxyfiring: A life-cycle perspective," AFRC International Pacific Rim Combustion Symposium, Maui, HI, September 26-29, 2010.

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

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

J. H. Bauman and M. D. Deo, “Parameter space reduction and sensitivity analysis in complex thermal subsurface production processes.” Manuscript submitted for review to *Energy and Fuels*.

I. S. O. Pimienta, A. M. Orendt, R. J. Pugmire, and J. C. Facelli , D. R. Locke, R. E. Winans, K. W. Chapman, and P. J. Chupas, “Three-dimensional structure of the Siskin Green River oil shale kerogen model: A computational study.” Publication of manuscript has been delayed pending acquisition of experimental data.

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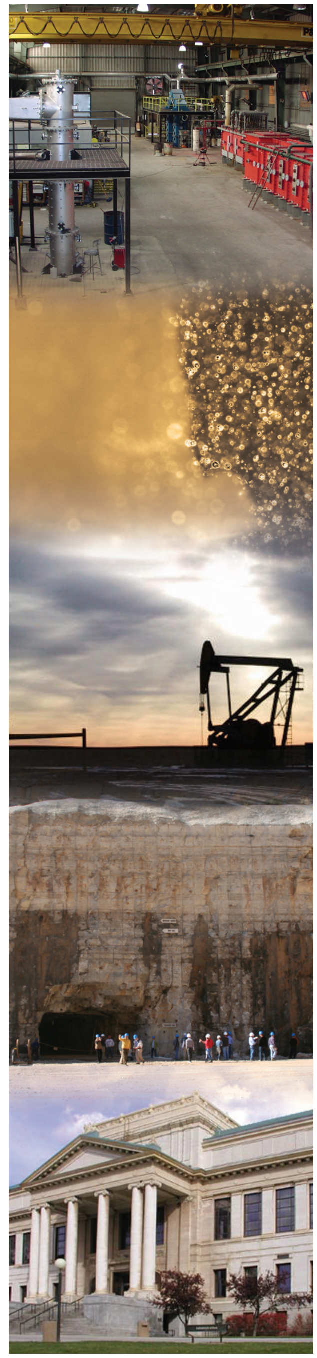
Lallemant, N.; Dugue, J.; Weber, R. Analysis of the experimental data collected during the OXYFLAM-1 and OXYFLAM-2 experiment, Phase 1: 1995-1996. IFRF Doc No F 85/y/4, International Flame Research Foundation, IJmuiden, The Netherlands (1997).

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

APPENDIX A. Agenda for Advisory Board Meeting

ADVISORY BOARD MEETING 2010



APRIL 27th

7:45 - 8:15 AM	Arrival and Breakfast
8:15 - 8:30 AM	Welcome and Introductions -Dave Pershing
8:30 - 9:15 AM	ICSE Overview -Phil Smith
9:15 - 9:30 AM	Break
9:30 - 12:00 PM	Research Presentations Kevin Whitty-Gasification Arnold Reitze-Sequestration James Sutherland-Mineralization
12:00 - 1:00 PM	Lunch
1:00 - 2:45 PM	Discussion of the "Demonstration Scale Question"
2:45 - 3:00 PM	Break
3:00 - 4:00 PM	Executive Session

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APPENDIX B. Agenda for University of Utah Unconventional Fuels Conference

AGENDA - APRIL 28th - 2010 UNCONVENTIONAL FUELS CONFERENCE: PRODUCTION OF FUELS FROM OIL SHALE, OIL SANDS AND COAL

8:30 - 8:50 AM — Welcome, New Initiatives - Dr. Philip J. Smith, Director, Institute for Clean & Secure Energy

8:50 - 9:15 AM — "Unconventional Fuels in the Uinta Basin: History and Current Efforts" - Mark Raymond, Uintah County Commissioner

9:15 - 9:40 AM — "Utah's Perspective on Unconventional Fuel Development" - Dr. Dianne Nielson, Energy Advisor to Governor Herbert for the State of Utah

9:40 - 10:10 AM — "Role of Unconventional Fuels in the Nation's Energy Portfolio" - Steve Black, Counselor to the Secretary, U.S. Department of the Interior

10:10 - 10:40 AM — Break, Core Workshop

RESEARCH ACTIVITIES

10:40 - 11:05 AM — "Underground Coal Gasification" - Dr. David C. Camp, Project Leader in Underground Coal Gasification, Lawrence Livermore National Laboratory

11:05 - 11:30 AM — "Enhanced In Situ Production through Fracturing" - Dr. John McLennan, USTAR Associate Professor, University of Utah

11:30 - 11:55 AM — "Geologic Characterization of Utah Oil Shale Deposits" - Dr. Lauren Birgenheier, Energy & Geoscience Institute & Institute for Clean & Secure Energy, University of Utah

11:55 - 12:20 PM — "Environmental Impact of the Oil Sands Development" - Dr. David Sego, Professor, Civil and Environmental Engineering, University of Alberta

12:20 - 1:30 PM — Lunch, Poster Session of Unconventional Fuels Research at the University of Utah, Core Workshop

INDUSTRIAL PERSPECTIVES

1:30 - 1:55 PM — "Shovel Ready...Can You Dig It?" - D. Glen Snarr, President & Chief Financial Officer, Earth Energy Resources

1:55 - 2:20 PM — "Status of OSEC's White River Oil Shale Project" - Gary Aho, Vice President of Operations, Oil Shale Exploration Company & Chairman, National Oil Shale Association

2:20 - 2:45 PM — "Update and Policy Considerations for Oil Shale Development" - Dr. Laura Nelson, Vice President of Energy & Environmental Development, Red Leaf Resources & Chair, Utah Mining Association Oil Shale/Tar Sands Committee

2:45 - 3:10 PM — "Progress and Plans on AMSO's RD&D Lease Tract" - Dr. Alan Burnham, Chief Technology Officer, American Shale Oil LLC

3:10 - 3:40 PM — Break, Core Workshop

PLENARY SPEAKER

3:40 - 4:15 PM — "Federal Control of Greenhouse Gas Emissions" - Arnold W. Reitze Jr., Professor, S.J.Quinney College of Law, University of Utah

The Utah Geological Survey will be exhibiting oil shale & oil sands cores during the morning, lunchtime & afternoon breaks.

Institute for CLEAN AND SECURE ENERGY
THE UNIVERSITY OF UTAH

Royalties and Taxes on Albertan Oil Sands Projects

Michael Hogue

This draft last updated July 29, 2010

1. Introduction

Policy-makers have a number of tools available which can and have been used with the intent to stimulate or curb certain types of economic activity. Because much of the oil and natural gas in the U.S. and Canada reside on public lands, tax and royalty arrangements that favor investment in exploration, development, and production of oil and gas are often deployed wherever it is believed that such activity is worthy of special incentives.

This section discusses economic arguments for and against particular royalty/tax treatments, with an emphasis on those which have been applied to the U.S. and Canadian oil industries. We describe the past and present royalty and tax regimes for Canadian oil sands projects, emphasizing what may be usefully gleaned from that experience.

2. The economic argument for special incentives

Economists generally believe that market prices provide appropriate incentives for producers and consumers. The most commonly acknowledged exception to this rule occurs when production or consumption entails a cost or benefit to one not directly involved in either. Incidental effects such as these are termed “externalities” because they are outside the scope of the (internal) cost-benefit considerations that take place between consumers and producers and which determines the level of production and consumption of the product at issue.

Pollution provides a classic example of a negative externality—an externality in which a cost, rather than a benefit, accrues outside the direct economic activity. A textbook on environmental and natural resource economics gives the following illustration:

> Suppose two firms are located by a river. The first produces steel, while the second, somewhat downstream, operates a resort hotel. Both use the river, though in different ways. The steel firm uses it as a receptacle for its waste, while the second uses it to attract customers seeking water recreation. If these two facilities have owners, an efficient use of the water is not likely to result. Because the steel plant does not bear the cost of reduced business at the resort resulting from waste being dumped into the river, it is not likely to be very sensitive to that cost in its decision making. As a result, it could be expected to dump too much waste into the river, and an efficient allocation of the river would not be obtained.[1]

From a point of view that regards the welfare of the resort owner equally with the welfare of the steel plant owner, the most efficient outcome is the one in which their

[1][See Tietenberg, Tom, *Environmental and Natural Resource Economics*, Addison-Wesley, 2000 p. 66.]

total welfare is maximized. This occurs only at a production level where the increment to total welfare of producing more steel is negative, while the increment to total welfare of producing less steel is positive.[2]

It has been advanced that although domestic fossil fuel production may entail certain public health and environmental negative externalities, these have to be weighed against a positive externality in the form of a reduced exposure to the macroeconomic risk of a sudden and unforeseen curtailment of oil supply, such as occured in late 1973.[3]

One way to move the status-quo level of production to a desired level is through fiscal policies that alter the price the product's producer recieves. A tax, for example, may be levied on product sales. Typically, although a portion of the tax will passed on to the consumer of the product, a significant portion will be borne by the producer. This has the effect of making production less attractive. One might consider such an action either because it is believed aggregate welfare would be increased at a lower level of production, or because it is believed that the gain in revenue from the remaining level of production is more than sufficient to offset the revenue lost from the production which is no longer forthcoming.

Although taxes and royalties each reduce the price a producer recieves and increase total "government take," they are motivated by different purposes. A royalty, but not a tax, is a return to the owner of the resource. Severance taxes in Utah, for example, are levied on all conventional oil and gas production within the state's geograhical boundaries, not just production occuring on state lands.

When an oil deposit is privately owned, it is expected the owner will set royalty terms they believe will maximize their share of the value created when the resource is developed. If the terms are too severe, resource development may be sufficiently curtailed that the share of value created flowing to the owner is less than what it could be under less severe terms. On the other hand, if the terms are too favorable, then less value flows to the owner than would under more severe terms. This is largely the same as the generic dilemma facing a firm that has to decide how to price its product.

3. Fiscal regimes applied to oil sands projects

Fiscal regimes bearing on oil sands projects can be divided into three periods. Although these periods correspond to specific and official rules governing royalties, they also relate well to three phases in the development of the oil sands industry. Policy with respect to oil sands projects has always been concerned with nurturing their development, in light of high costs and special risks. However, as development has advanced (e.g. production costs have decreased and special risks somwhat abated) concern has increasingly turned

[2]Welfare includes both private and external costs and benefits.

[3]Conceptual issues in this "energy security externality" are thoroughly discussed in: [Toman, Michael A. and Bohi, Douglas R., *The Economics of Energy Security*, Springer, 1996].

toward extracting more of the value of oil sands production for the public.[4,5]

3.1. BEFORE 1997 The commerical beginning of the oil sands industry is marked by initial production (in 1967) from what is now the Suncor Energy company, following decades of basic research and the support of the Albertan government.[6] Following Suncor in commerical operation was Syncrude, which came online in July 1978. As of the early 1990's only a few commercial oil sands projects were operating: Suncor, Syncrude, and a small number of in situ projects.

During this early stage of development, royalties were set by case-by-case agreements with the Crown, rather than legislation. Royalty rates ranged from 1 to 5 percent on gross revenue and 25 to 50 percent on net revenue.[7] Both Suncor and Syncrude had royalty agreements which called for revenue calculations based on the price of synthetic crude oil, rather than the much cheaper raw bitumen.[8,9] (Plourde, 2009) notes that in the mid-1980s a number of large projects were either cancelled or postponed over concerns which included lack of a certain royalty regime. When evaluating potential developments, investors could not know what royalty regime they would ultimately face, that could only be decided at a more advanced stage of planning.

In 1993 the National Task Force on Oil Sands Strategies was formed between members of industry and government. The purpose of the Task Force was to determine what policies could be undertaken to spur on oil sands industry. In 1995 the Task force delivered, and the Albertan government accepted, its recommendation that royalty provisions be uniformly applied rather than applied through individual agreements with the Crown. This new regime, known as the Generic Oil Sands Royalty Regime (GOSRR), began in late 1997.

According to (Alberta Energy, 1998), the objective of the new system was twofold[10]:

[4][Plourde, André, Oil Sands Royalties and Taxes in Alberta: An Assessment of Key Developments since the mid-1990s, THE ENERGY JOURNAL 30 2009, Nr. 1] notes that Alberta recieves four types of payments from oil sands development: bonus bids—winning bids on the right to develop offered sites (1.112 billion in 2008/2009, down from 2.463 billion in 2006/07 [Government of Alberta]), rental fees (C$3.50 per hectare per year; 160 million in 2008/09), royalties (2.973 billion in 2008/09), and provincial corporate income taxes (in addition to the corporate income tax levied by the Canadian federal government). Royalties are deductible from Canadian federal income tax.(Kayande, 2006).

[5]The Albertan government ("the Crown") owns 81 percent of mineral rights [energy economics, p.6], but owns 97 percent of oil sands mineral rights. The remainder is owned by freeholders. [oil sands royalty guidlines Ch. 1, p.1]

[6][See Congression Research Service, *North American Oil Sands: History of Development, Prospects for the Future*, 2008 January].

[7][See Goverment of Alberta, *Alberta Oil Sands Royalty Guidlines, Chapter 1: Alberta's Oil Sands Royalty System*, 2006 November p. 1].

[8]"Alberta's bitumen has been worth 26 per cent to 80 per cent of WTI during [the four years ending 2009] recognizing the upgrading, refining and transportation costs in creating higher value products from oil sands crude."[See Government of Alberta, *Energy Economics: Understanding Royalties*, September 2009 p. 9].

[9]These agreements expired in 2009 and have been replaced with interim agreements which are in effect until 2016, at which point both Suncor and Syncrude will fall under the current royalty regime.

[10][See Alberta Energy, *Information Letter 98-3*, January 1998 p. 2].

> To establish a single, clear and stable royalty regime that is applicable to all new investments in oil sands and facilitates development without the Province of Alberta having to provide grants, loans, loan guarantees, or become directly involved in any capacity other than resource owner.

and

> To ensure that oil sands development in Alberta is generally competitive with other petroleum development investment opportunities around the world.

Among others, the provisions of the new regime included requirements for project approval, royalties based on net revenue (as before) and definitions of costs which could be deducted from gross revenue for the purposes of estimating whether a project had reached payout.

3.2. BETWEEN 1997 AND 2007 The government of Alberta initiated the "Generic Oil Sands Royalty Regime" (GOSRR) in 1997, ending the period in which royalties for oil sands operations were negotiated on a case-by-case basis. Under the 1997–2007 regime, producers could choose whether to base royalties on bitumen production or synthetic crude oil production (SCO).[11] If they chose to base royalties on bitumen production, then the allowable costs would not include capital (including return on investment) or operating costs for upgrading, and allowable revenue would be based on bitumen prices, rather than SCO prices.

Under GOSRR, for each oil sands project royalties were 1 percent of gross revenue until the project reaches "payout."—the date when cumulative revenue from the project equals cumulative costs. Among the allowable costs is a return on ivestment, which is set at the Goverment of Canada long-term bond rate (about 4 percent as of July 2010). That is, reaching payout means recovering costs and making a conventional profit. After reaching payout, royalties are either 1 percent of gross revenue or 25 percent of net revenue, whichever is greater. This risk-sharing arrangment is meant to encourage and support new projects until they have returned their investor's costs plus a return. [12]

3.3. SINCE 2007 By the mid-2000s, oil prices had risen well above the level that prevailed near the time of the 1997 regime change. Oil sands production nearly doubled between 1997 (30,604 thousand cubic meters) and 2005 (57,550 thousand cubic meters). This led to a growing belief that the 1997 regime had already become outdated. This led the Albertan government to commission the Albert Royaly Review Panel to consider alternative fiscal regimes.

The Panel's findings, released in 2007, were stark, claiming: "Albertans do not receive their fair share from energy development."(See Alberta Royalty Review Panel, 2007, p. 7).

[11]SCO is bitumen that has undergone "upgrading"—processes that generally render a product physically similar to conventional refinery feedstock. Upgrading can be regarded as "pre-refining."

[12]As of February 2009, 48 oil sands project were in pre-payout and 43 were in post-payout.[See Government of Alberta, *Energy Economics: Understanding Royalties*, September 2009 p. 14].

The Panel argued that the total government take from oil sands projects, in light of the then-present royalty structure and oil prices were favorable compared to projects in other parts of the world, and could withstand an increase without significantly curtailing development:

> The total government take (Alberta and Canada, taxes and royalties) can be increased with Alberta still remaining an attractive investment destination. (See Alberta Royalty Review Panel, 2007, p. 7).

and

> Cumulatively, the Panel's recommended package of changes for oil sands targets a total government take from the oil sands sector of 64%, increased over the present total take which is a little under 50%. Roughly 60% was the total take level identified by the 1995 National Oil Sands Task Force (NOSTF) as consistent with the needs of a fledgling industry. The Panel regards a comparable level of take as more than reasonable for the production powerhouse the sector has become.(See Alberta Royalty Review Panel, 2007, p. 11)

Following the Panel, a new royalty regime was implemented "The New Royalty Framework." The new royalty framework retains the previous regime's differential treatment between pre and post-payout projects. For pre-payout projects, the royalty is still 1 percent of gross revenue while the price of West Texas Intermediate (WTI) is less than C$56/bbl. However, when WTI is at or above C$56/bbl, the royalty is 1 percent of gross revenue and an additional 0.12308 percent of gross revenue for every dollar the price of WTI is above $55/bbl but not more than $120/bbl. At $120/bbl (and beyond), the applicable royalty rate is 9 percent $(0.01+(120-55)\times\ 0.12308)$ of gross revenue. In the post-payout period, royalty rates are 25 percent of net revenue while the price of WTI is less than $56 and increases by 0.23077 percent for every dollar it is at or above $56/bbl but below $120/bbl. Thus, post-payout royalty rates on net revenue range from a 25 to 40 percent.

For Suncor, in-situ projects became subject to the new regime beginning in 2009. While Suncor's mining operations don't come under the new regime until 2016, due to an agreement with the Albertan gov't that pre-dated the new royalty famework (and its predessor). Until 2016, Suncor's royalties will be based on bitumen prices instead of on SCO.

4. U.S. fiscal regime for oil production

The U.S. federal government does not yet have a fiscal regime in place for domestic oil sands. In Utah, where a majority of the domestic oil sands resource is located, the royalty regime for production on state lands is the same as for conventional oil and gas. Oil sands production is exempt from the state severance tax at least until this provision expires in 2016. For typical oil projects in Utah (not low-production wells) the severance tax is 3 percent of the sales price while the price is less than $13/bbl and increases to 5 percent of sales for the portion of sales price above $13/bbl.

Of U.S. oil resources, the most comparable to the Canadian oil sands is probably deep-water offshore and California heavy oil.

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Prices for Project Valuation

Michael Hogue

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1. Overview

Our scenarios are "oil projects"—operations deriving nearly all of their revenue from the production and sale of crude oil (or a close substitute). Oil prices along the 20-year lifetime we have assumed for these projects are therefore a critical factor in their commercial success. For this reason we measure and report the profitability of the scenarios along a range of possible futures price paths. In this section we discuss the price forecasts we have used for this purpose.

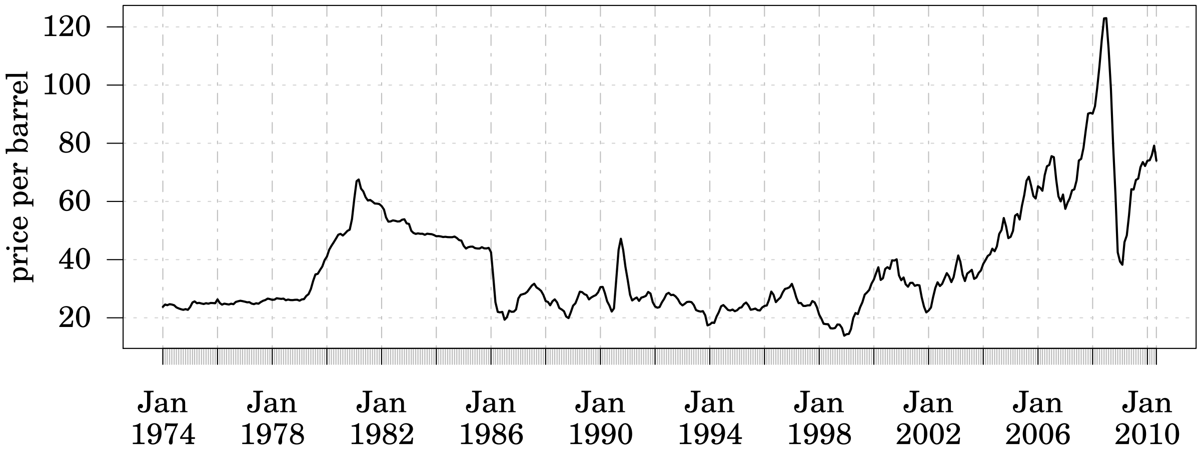

Figure 1: U.S. refiner's acquisition price of domestic crude measured in September 2009 dollars. In the last 20 years oil prices have ranged from $47/bbl in October 1990—following the August 1990 invasion of Kuwait by Iraq—to $14/bbl by the end of 1998 due to an untimely production quota increase by OPEC in the wake of the Asian economic crisis, to an all-time high of $123 in July 2008, down to $74/bbl in May 2010. The average oil price since May 1990 is $40/bbl in Sept. 2009 dollars.

2. Forecasts from the EIA's Annual Energy Outlook (2010)

Each year the Energy Information Administration (EIA) of the U.S. Department of Energy prepares 25-year forecasts for a given set of energy variables, along with forecasts of certain particularly important macroeconomic variables. These forecasts are published as part of the the EIA's Annual Energy Outlook (AEO) (U.S. Energy Information Administration, 2010).[1]

[1]The tool EIA employs for this purpose is the National Energy Modelling System (NEMS). NEMS is a computable general equilibrium model—a set of mathematical relations meant to desribe the economy and interaction among its economic actors. The forecasts from NEMS are the responses necessary to re-establish an assumed equilibrium among the relations (e.g. so that supply and demand continue to balance) following some set of external changes. See http://www.eia.doe.gov/oiaf/aeo/overview/.

For each variable there are typically three forecasts: a reference case, a low case, and a high case. The following excerpt from the current AEO discusses the nature of such forecasts (see U.S. Energy Information Administration, 2010, p. ii.).

> Projections by EIA are not statements of what will happen but of what might happen, given the assumptions and methodologies used for any particular scenario. The Reference case projection is a business-as-usual trend estimate, given known technology and technological and demographic trends. EIA explores the impacts of alternative assumptions in other scenarios with different macroeconomic growth rates, world oil prices, and rates of technology progress. The main cases in AEO2010 generally assume that current laws and regulations are maintained throughout the projections. Thus, the projections provide policy-neutral baselines that can be used to analyze policy initiatives.

Note that, in particular, the AEO cases do not reflect possible impacts from CO_2 regulation, as such regulations are not yet established.

In addition to cases based on broad economic considerations, the AEO provides regionalized forecasts for energy variables. For our scenario projects located in the Rocky Mountain region, we used the AEO "Mountain" region forecasts for both the price of electricity for industrial customers and the delivered price of natural gas.[2] Rather than use the regional forecasts for oil prices, we use forecasts for the national refiner's aquisition cost of imported low sulfur light crude.

3. Stochastic Price Models

The EIA forecasts, based on the National Economic Modelling System, are not statistical. Hence, they do not come with conventional prediction intervals or any other measure of forecast uncertainty quantified with probability distributions. Instead, the EIA forecasts deal with uncertainty by applying the NEMS model to a set of plausible scenarios, rather than just one.

In this section we discuss several popular models for commodity prices—in this case oil—in which the apparent randomness of price is explicitly modelled. For each of these models, we use historical prices to estimate it's parameters, provide probability distributions (keyed to these parameter estimates as well as to the model) for price at every future date in our forecast horizon (20 years), provide the corresponding simulation models, and supporting technical detail.

Th simulation models take the general form of generating at every time t a price which is a function of price in the immediately previous period only and a contemporaneous random distrubance (see equations (7) and (19) below). We calibrate the parameters

[2] For electricity, the regional forecasts are only given in dollars per million BTUH. We convert from BTUH to KWH using the factor: 1 KWH per 3412 BTUH. This conversion factor is calculated from the national price forecasts, which are given in both BTUH and KWH units. For natural gas, we convert from price per thousand cubic feet (Mcf) to price per million BTU (MMBTU) using the conversion factor: 1 MMBTU per 1.031 Mcf.

of each model with statistical estimates based on monthly values of the “U.S. Crude Oil Domestic Acquisition Cost by Refiners” since 1974.

3.1. Geometric Brownian Motion Denote the price of oil at time t by “$P(t)$.” Then $\mathrm{d}P(t)$ is the change in price in the interval t to $t+\mathrm{d}t$, where $\mathrm{d}t$ is a very small positive number.

Then $P(t)$ is said to follow a geometric Brownian motion (GBM) if it satisfies:

$$\mathrm{d}P(t) = \mu P(t)\,\mathrm{d}t + \sigma P(t)\,\mathrm{d}z(t). \tag{1}$$

Note that the drift and volatility terms are proportional to the price level in the GBM model. A fundamental result in stochastic calculus, Itô’s Lemma, can be employed to show that (1) implies

$$\mathrm{d}\log P(t) = (\mu - \sigma^2/2)\,\mathrm{d}t + \sigma\,\mathrm{d}z(t). \tag{2}$$

Equation (2) then implies (see Gourieroux and Jasiak, 2001, p. 287):

$$\Delta \log P(t) = \mu - \sigma^2/2 + \sigma\varepsilon(t) \tag{3}$$

Thus, if price follows the geometric Brownian motion given in (1), then the natural logarithm of price follows an arithmetic brownian motion, which has the general form that the drift and volatility terms are constants, rather than proportional to levels of the variable. Importantly, (2) says that (instantaneous) percentage changes in price, rather than price itself, follow a continuous random walk with drift. The implication is that in this model price remains positive with certainty.

Let $m \equiv \mu - \sigma^2/2$. The maximum likelihood estimators for m and σ^2 are

$$\hat{m} \equiv \frac{1}{T}\sum_{t=1}^{T} \Delta \log P(t), \quad \hat{\sigma}^2 \equiv \frac{1}{T}\sum_{t=1}^{T} \left(\Delta \log P(t) - \hat{m}\right)^2, \quad \hat{\mu} = \hat{m} + \hat{\sigma}^2/2. \tag{4}$$

Under the GBM model, for times $s < t$, $[P(t)\,|\,P(s)]$ is lognormally distributed with parameters $\log\ P(s) + (t-s)\left(\mu - \frac{\sigma^2}{2}\right)$ (the “log-mean”) and $t\sigma^2$ (the “log-variance”). Further, the conditional expected value, $\mathrm{E}[P(t)\,|\,P(s)]$, is $P(s)e^{\mu(t-s)}$ and conditional standard deviation, $\mathrm{SD}[P(t)\,|\,P(s)]$, is $P(s)e^{\mu(t-s)}\left(e^{\sigma^2(t-s)} - 1\right)^{\frac{1}{2}}$, where $P(s)$ is a given price (Dixit and Pindyck, 1994). In particular, for all times t,

$$\mathrm{E}[P(t)\,|\,P(t-1)] = P(t-1)e^{\mu}, \quad \mathrm{SD}[P(t)\,|\,P(t-1)] = P(t-1)e^{\mu}\left(e^{\sigma^2} - 1\right)^{\frac{1}{2}}. \tag{5}$$

$$\left(P(t)\,|\,P(s)\right) \sim \mathrm{LN}\left(\log\ P(s) + (t-s)\left(\mu - \frac{\sigma^2}{2}\right), (t-s)\sigma^2\right) \tag{6}$$

To simulate the price at any future time t, starting from some initial time $s := t_0$, we draw a lognormal (psuedo) random variable with the parameters given above.

Though we can do this in arbitrarily fine increments, the sequence of prices resulting from such a sequence of draws is not a path. To simulate paths for GBM, we use the discretized form of equation (1) (see Dixit and Pindyck, 1994, p. 72):

$$P_t = (1+\mu)P_{t-1} + \sigma P_{t-1}\varepsilon_t, \tag{7}$$

where ε_t is a standard normal random variable. Inserting the estimates of μ and σ from Table 1, we obtain the following calibrated models:

$$P_t = 1.004714 * P_{t-1} + 0.06492 * P_{t-1}\varepsilon_t. \tag{8}$$

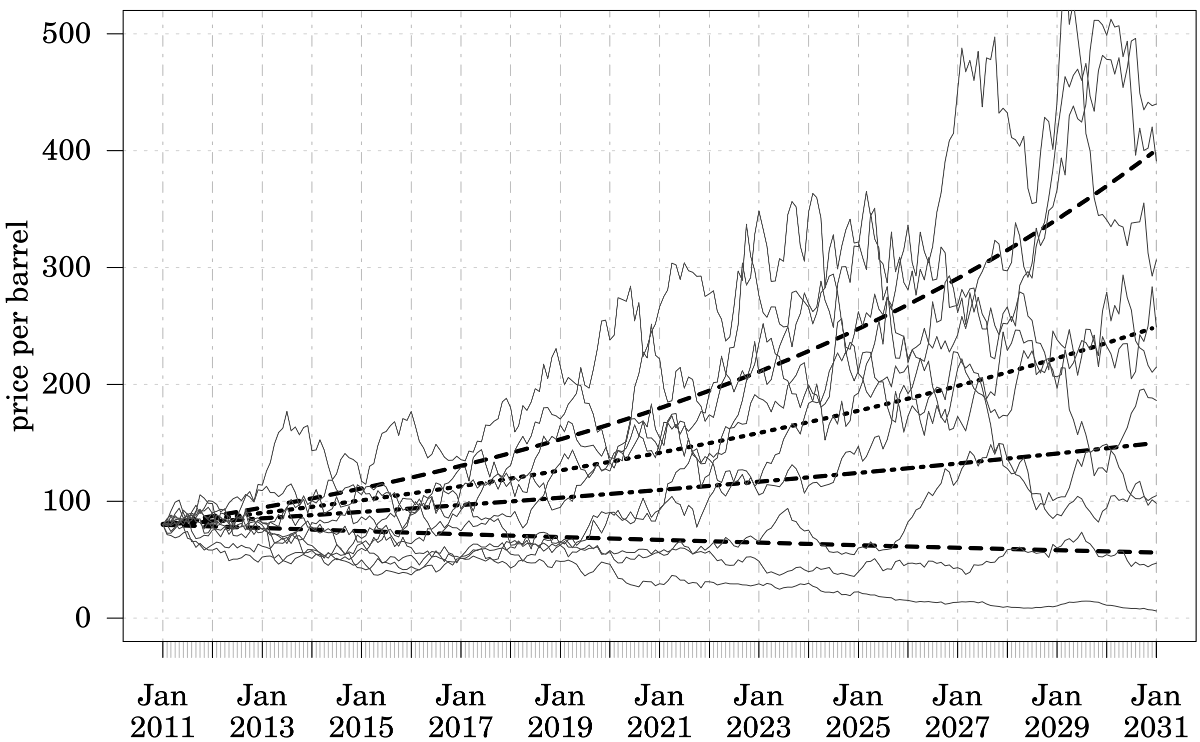

Figure 2: Ten 20-year sample paths are shown from the calibrated GBM model (light grey). The upper and lowermost lines (dashed) are the 83.3% and 16.7% bounds for the price paths. The lower of the two middle lines is the median price path (dot-dashed) and the upper of the two middle lines is the expected (mean) price path. At every time t, the prices have a lognormal distribution with parameters depending on t.

3.2. REVERSION TO A CONSTANT MEAN Compared with GBM, models which endow prices with a tendency to an equilibrium value are often seen as less in conflict with accepted economic and financial theory. Such a class of models is usually denoted "mean-reverting"—GBM models imply prices that are mean-*averting*—or Ornstein-Uhlenbeck models, in recognition of the physicists Leonard Ornstein and George Uhlenbeck whose work in the 1930s on gas kinetics employed a simple mean reverting model.

A simple and widely used model with reversion to a constant mean (MR) is the following:

$$\mathrm{d}P = \lambda\left(\bar{P} - P(t)\right)\mathrm{d}t + \sigma\,\mathrm{d}z, \tag{9}$$

where $\lambda \geq 0$ is the rate of reversion of the instantaneous price $P(t)$ to the equilibrium price $\bar{P}$. Equation (9) implies that price changes are negative (positive) whenever $P(t)$ is greater (lesser) than $\bar{P}$. Further, the absolute value of the price change is a constant proportion of the deviation of $P(t)$ from $\bar{P}$: The farther (closer) in absolute value is $P(t)$ from $\bar{P}$, the more likely is a large (small) change in price in the direction of $\bar{P}$.

If P_0 is the current price, then the conditional expected value and variance of price t time units in the future are (see Dixit and Pindyck, 1994, pp. 74–75 and Appendix A pp. 90–91)

$$\mathrm{E}[P_t|P_0] = \bar{P} + \left(P_0 - \bar{P}\right)e^{-\lambda t}, \tag{10}$$

and

$$\mathrm{V}[P_t|P_0] = \frac{\sigma^2}{2\lambda}\left(1 - e^{-\lambda t}\right). \tag{11}$$

The discretized version of (9) is

$$P_t = \bar{P}\left(1 - e^{-\lambda}\right) + P_{t-1}e^{-\lambda} + \sigma\varepsilon_t\left(\frac{1 - e^{-2\lambda}}{2\lambda}\right)^{1/2}, \tag{12}$$

with ε_t a standard normal random variable.

Equation (12) is the autoregressive time series model $P_t = \bar{P}\,(1-\beta) + \beta P_{t-1} + \phi\varepsilon_t$, where $\beta = e^{-\lambda}$ and $\phi = \sigma\left(\frac{1-\beta^2}{2\log\beta}\right)^{1/2}$. The following are the maximum likelihood estimators for β, $\bar{P}$, ϕ, λ, and σ^2 (see Gourieroux and Jasiak, 2001, p. 290):

$$\hat{\beta} \equiv \frac{\sum_{t=1}^{T}\left(P_t - \bar{P}\right)\left(P_{t-1} - \bar{P}\right)}{\sum_{t=1}^{T}\left(P_t - \bar{P}\right)^2}, \tag{13}$$

$$\hat{\bar{P}} \equiv \frac{1}{T}\sum_{t=1}^{T} P_t, \tag{14}$$

$$\hat{\phi}^2 \equiv \frac{1}{T}\sum_{t=1}^{T}\hat{\varepsilon}_t^2 \equiv \left[P_t - \hat{\bar{P}} - \hat{\beta}\left(P_{t-1} - \hat{\bar{P}}\right)\right]^2, \tag{15}$$

and, using the definitions of β and ϕ,

$$\hat{\lambda} \equiv -\log \hat{\beta}, \tag{16}$$

$$\hat{\sigma}^2 \equiv \frac{-2\log \hat{\beta}}{1-\hat{\beta}^2}\hat{\phi}^2. \tag{17}$$

Of particular note is that the estimator $\hat{\beta}$ is the same as the 1st order sample correlation—the correlation between P_t and P_{t-1} as calculated from data at hand—and $\hat{\bar{P}}$ is simply the sample average price. Substituting the parameter estimates (see Table 2) into equations (9) and (12) gives

$$\mathrm{d}P = 0.0147\left(37.8254 - P(t)\right)\mathrm{d}t + 2.9044\,\mathrm{d}z, \tag{18}$$

while doing the same for the short form of (12) gives:

$$P_t = \bar{P}\left(1-\beta\right) + \beta P_{t-1} + \phi\varepsilon_t \tag{19}$$

$$= 37.82546(1-0.9853738) + 0.9853738 P_{t-1} + \sqrt{8.312932}\varepsilon_t$$

$$= 0.5532426 + 0.9853738 P_{t-1} + 2.883216\varepsilon_t. \tag{20}$$

3.3. Reversion to a linear trend If we consider that price is attracted to an underlying average price that is increasing linearly with time rather than remaining constant, Then the setup is the same as with the MR model but we first use the data to estimate the linear time trend before apply MR to the detrended data. The parameter estimates are given in Table 3. In the simulation model and price distributions the constant mean of the MR model is replaced with the estimated time trend $\hat{a} + \hat{b}t$.

4. Data and Calculations

We put together a file named "oil.csv," which contains information arranged in four columns. The last three columns hold data on the "Monthly U.S. Crude Oil Domestic Acquisition Cost by Refiners" (column two), the "Producer's Price Index" ("PPI," column three), and the "Inflation-adjusted Monthly U.S. Crude Oil Domestic Acquisition Cost by Refiners" (column four) which is computed from columns two and three.[3] The first column holds the dates (January 1974 through May 2010) for this data. Values for the PPI were obtained from the Bureau of Labor Statistics.[4] The oil prices were obtained from the Energy Information Administration of the U.S. Department of Energy.[5]

[3] Denoting the value of the PPI at date t by "I_t," and the nominal acquisition cost at date t by "N_t," the inflation-adjusted acquisition cost, denoted "R_t," is calculated as: $R_t = N_t\left(\frac{I_T}{I_t}\right)$, where T is the basis date.

[4] See http://www.bls.gov/data/.

[5] See http://www.eia.gov/dnav/pet/pet_pri_rac2_dcu_nus_m.htm.

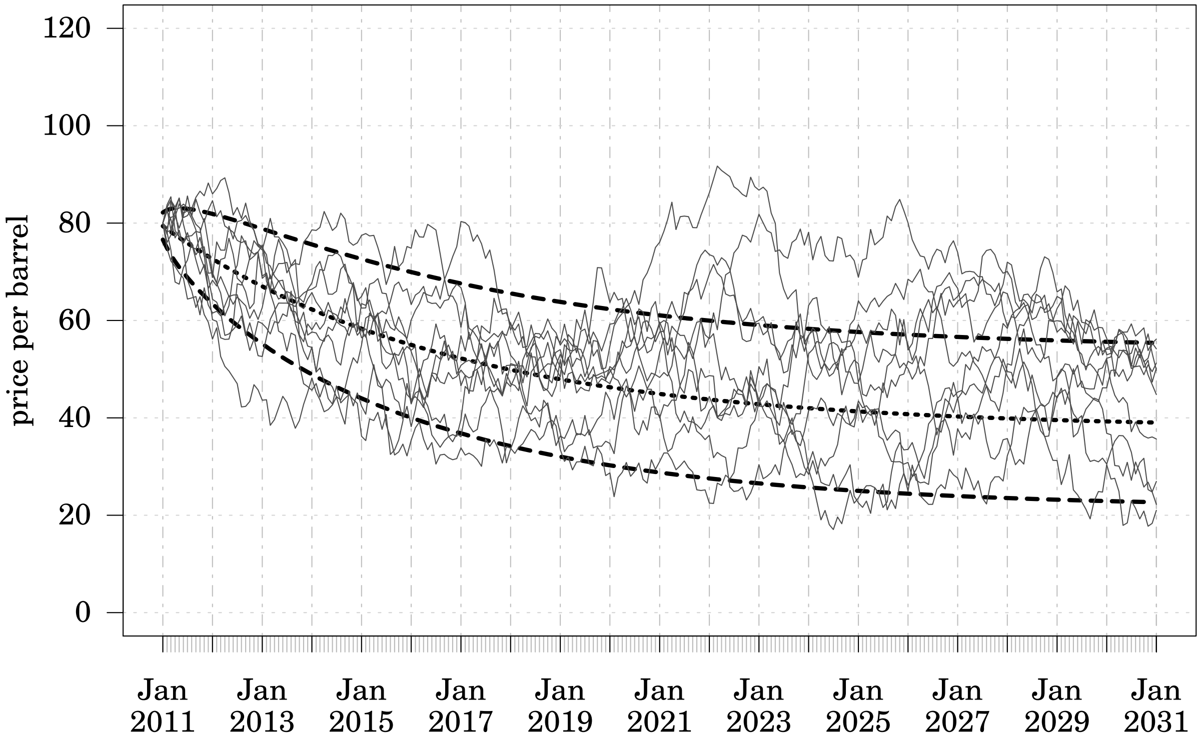

Figure 3: Ten 20-year sample paths are shown from the calibrated MR model (light grey). The upper and lowermost lines (dashed) are the 83.3% and 16.7% bounds for the price paths. The middle line (dotted) is the expected (mean) price path. In this case, unlike that of GBM, the median and expected price paths are the same. At every time t, the prices have a normal distribution with parameters depending on t.

References

[1] Dixit, Avinash K. and Pindyck, Robert S., *Investment Under Uncertainty*, Princeton University Press, 1994

[2] Gourieroux, Christian and Jasiak, Joann, *Financial Econometrics*, Princeton University Press, 2001

[3] U.S. Energy Information Administration, *Annual Energy Outlook 2010*, 2010 – Technical report

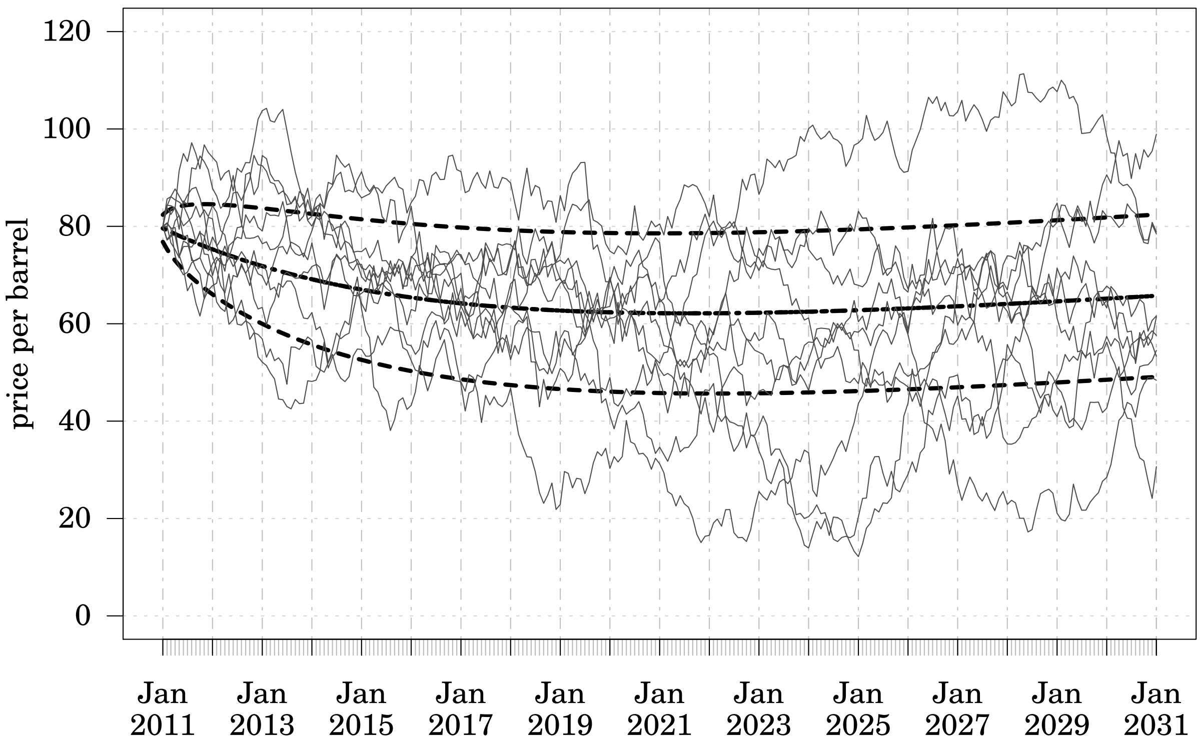

Figure 4: Ten 20-year sample paths are shown from the calibrated TMR model (light grey). The upper and lowermost lines (dashed) are the 83.3% and 16.7% bounds for the price paths. The middle line (dotted) is the expected (mean) price path. In this case, unlike that of GBM, the median and expected price paths are the same. At every time t, the prices have a normal distribution with parameters depending on t.

parameter	estimate
$\hat{m}$	0.002606366
μ	0.004713862
σ^2	0.00421499

Table 1: Estimates of the GBM parameters using inflation-adjusted (year 2009) prices.

parameter	estimate
$\hat{\beta}$	0.9853738
$\hat{\bar{P}}$	37.82546
$\hat{\phi}^2$	8.312932
λ	0.01473421
σ^2	$(2.904482)^2$

Table 2: Estimates of the MR parameters using inflation-adjusted (year 2009) prices.

parameter	estimate
$\hat{a}$	25.04967
$\hat{b}$	0.05860457
$\hat{\mu}$	0
$\hat{\beta}$	0.9859814
$\hat{\phi}^2$	8.271906
$\hat{\lambda}$	0.01411774
$\hat{\sigma^2}$	$(2.896418)^2$

Table 3: Estimates of the TMR parameters using inflation-adjusted (year 2009) prices.

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