Oil & Natural Gas Technology

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

Quarterly Progress Report (September - December 2011)

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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. The Clean and Secure Energy program hosted an External Advisory Board on November 1-2, 2011 and the kickoff meeting with industrial partner American Shale Oil (AMSO) on October 25, 2011 for the Strategic Alliance Reserve (SAR) projects.

Researchers in Task 3.0 are developing a modified assessment tool for evaluating regional economic and environmental effects of unconventional fuel development. In order to achieve this goal, researchers have created a module within the assessment tool framework for conventional oil and gas development in the Uinta Basin that include drilling schedules, well depth distributions, and production curves. They have also collected greenhouse gas and criteria pollutants emissions data as a prelude to developing an air emissions module. Data obtained from the Utah Division of Oil, Gas, and Mining (DOGM) and from other sources will be used for model validation/uncertainty quantification (V/UQ). This approach is being used due to the lack of unconventional fuel data available for V/UQ.

Subtask 3.2 researchers are focusing on developing a flamelets reaction/mixing model that can be coupled to Large Eddy Simulation (LES) codes to model subgrid scale reaction and mixing processes. This flamelets model will be used in the parametric study of the International Flame Research Foundation (IFRF) oxy-fuel-fired furnace. Stability problems with the IFRF furnace geometry and boundary conditions in the LES code ARCHES have slowed down efforts to complete a V/UQ analysis of this system.

Research and analyses on three different sections of the Skyline 16 core (GR-1, GR-2, and GR-3) was the focus of Subtasks 4.3, 4.5, 4.6, and 4.9 during this quarter. The Subtask 4.3 has completed thermogravimetric analysis (TGA) pyrolysis of demineralized kerogen that has extracted from Gr-1, GR-2, and GR-3. For all three kerogens, onset points (start and end) in the pyrolysis zone are close to identical. In Subtask 4.5, researchers analyzed the GR-1, GR-2, and GR-3 samples before and after pyrolysis. The images reconstructed from X-ray computed tomography (CT) show that pores are generated along the kerogen-rich layers in the GR-1 sample while directional fractures along the thin, kerogen-rich layers are observed for GR-2 and GR-3 samples. Work in Subtasks 4.6 and 4.9 are focused on providing models for oil shale kerogens and experimental data for model validation. The Subtask 4.6 team studied the effect of the interaction of organic materials (e.g. kerogen) with inorganic materials on the nuclear magnetic resonance (NMR) spectrum and obtained both ^{13}C SSNMR and pairwise distribution function (PDF) measurements on the kerogens isolated from the three core sections. Subtask 4.9 researchers verified through ashing tests that the demineralized kerogen samples used in Subtasks 4.3 and 4.6 had a mineral content of about 5%. Structural and lattice parameters have been extracted from the cross polarization (CP) and single pulse (SP) magic angle spinning (MAS) spectra, revealing that the organic matter in all three kerogen samples is similar. Subtask 4.7 will also be performing in-situ stress tests on the same section of oil shale cores once the apparatus is fully designed and evaluated. Design during this quarter focused on the internal measurement systems, specifically the measurement of axial and radial deformation of the samples while they are being tested.

The other Task 4.0 projects have focused on simulation of various in situ processes. Subtask 4.1 researchers have completed a topical report on heat transfer processes inside the representative computational geometry used for an evaluation of Red Leaf Resources' ECOSHALE capsule technology. They have also implemented a more complex geometric representation of the fractured oil shale bed by using two distinct particles in contact to represent three shapes and by decreasing the size of the convective channels. The Subtask 4.2 team has proposed a sequential combination of in situ pyrolysis, in situ combustion, and CO_2

enhanced oil recovery (EOR) to increase recovery of unconventional fuels while increasing production energy efficiency. They have evaluated the effect of time for switching from in situ pyrolysis to in situ combustion on overall production and energy supplied. Work on Subtask 4.8 was suspended this quarter due to the PI's maternity leave.

Subtask 5.0 researchers have completed two topical reports, one on conjunctive water management (already submitted) and the other on cross-jurisdictional resource management (to be submitted next quarter). In Task 6.0, the project team has determined that a two-pronged approach to profitability analysis in the Market Assessment is needed: the Supply Price Method and the Net Present Value Method. The four unconventional fuel development scenarios are being updated to reflect these changes. Additionally, five sections of the Market Assessment report have been completed in page layout form and are ready for publication after final proofing. The remaining five sections are being laid out at the rate of one section per week.

The three SAR subtasks were officially launched at the project kickoff meeting with AMSO. Initial work in Subtask 7.1 is focused on collecting information in the public domain on constitutive mechanical and thermal properties of oil shale. A data analysis specialist is being consulted in order to assess the best methodology for processing large volumes of experimental data. Subtask 7.3 researchers have used the HPC-based tools developed for Subtask 4.1 to create a preliminary simulation of a three-day heating process for a computational domain more representative of the AMSO process.

PROGRESS, RESULTS, AND DISCUSSION

Task 1.0 - Project Management and Planning

During this quarter, the PMP was amended to reflect the three new subtasks added under Task 7.0. The additional milestones under this task are included in the "Milestone" section of this report.

Task 2.0 -Technology Transfer and Outreach

Task 2.0 focuses on outreach and education efforts and the implementation of External Advisory Board (EAB) recommendations. During this quarter, Madhava Syamlal of NETL accepted ICSE's invitation to join the EAB and the EAB held its annual meeting on November 1-2, 2011. EAB members in attendance at the meeting were Ian Andrews of PacifiCorp; James Holtkamp of Holland & Hart; Robert Lestz of GasFrac; Dianne Nielson, formerly the Governor's Energy Advisory for the State of Utah; Laura Nelson of Red Leaf Resources; David Pershing, Distinguished Professor and Senior Vice President for Academic Affairs at the University of Utah and Director of the EAB; Mark Raymond, Uintah County Commissioner; and Adel Sarofim, Presidential Professor at the University of Utah. A copy of the materials distributed at the 2011 EAB meeting is attached as Appendix A. Recommendations from the meeting will be circulated for EAB approval next quarter.

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

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

Completion of the Phase 1 milestone is still delayed while results for the four oil shale and oil sands development scenarios are completed. Subtask 3.1 researchers anticipate receiving updated results by the end of February and expect to complete this task by March 2012.

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

During this quarter, the team continued to refine their understanding of oil and gas operations in the Uinta Basin, to collect relevant greenhouse gas (GHG) emission factors, and to understand both the AnyLogic software platform and the modules being developed on that platform. Some time was devoted this quarter to assisting Subtask 3.3 with collection of data from drilling reports including costs, well depth, and fuel usage. Some of this data will be important to the GHG emission modules.

Several potentially useful GHG sources for validation data will be released in the coming months, including the Bureau of Land Management's air emissions inventory and the Uinta Basin air emissions inventory update being developed by Utah State University. The research team continues to monitor the progress of these upcoming data sources.

During this quarter, efforts focused on developing transportation-related emission factors for the oil and gas air quality module. The estimates of criteria pollutants and GHGs from mobile sources are based on a US Environmental Protection Agency (EPA) study of transportation emissions associated with onshore oil and gas development in the Piceance Basin of Northwestern Colorado (EPA, 2011). This study builds on several inventory projects that have examined emissions from oil and gas development activities both in the Piceance Basin and in the Intermountain West generally. The investigators surveyed operators regarding off-road equipment and on-road vehicles used for various phases of oil and gas production, including well construction, well drilling, well completions (including fracturing), and production operations. The survey responses represented 63% of well ownership in the basin, 65% of gas production in the basin, and 78% of oil production in the basin.

All of the emissions are normalized based on spud counts or well counts in the 2009 base year (EPA, 2011). Spud and well counts are not differentiated between oil and gas. The EPA study only provides criteria-pollutant emission factors. Therefore, the research team estimated the mass of diesel fuel consumed using the total sulfur emissions, the sulfur content of the fuel, and the sulfur emission factors:

$$D = SO_2 \times \frac{MW_S}{MW_{SO_2}} \times \frac{1}{X} \quad (1)$$

where,
D = mass of diesel fuel
SO_2 = mass of sulfur emissions
X = Fuel sulfur content; for diesel, S content = 351 ppm (EPA, 2009) or 7.67×10^{-4} weight fraction; for gasoline, S content = 4.39×10^{-4} weight fraction
MW_s = Molecular weight of sulfur = 32.07
MW_{SO2} = Molecular weight of sulfur = 64.07

As part of this estimate, the diesel fuel density was assumed to be 0.832 kg/l and the ratio of the SO_2 emission factors for diesel and gasoline engines while idling were used.

For some activities, both gasoline and diesel fuel were consumed; therefore, Subtask 3.1 researchers had to apportion the annual emissions between gasoline and diesel fuels as shown in Equations (2) and (3):

$$X_{SO_2-idle} = \frac{(RT \times Idle_{hr} \times EF_{SO_2})_{Diesel}}{(RT \times Idle_{hr} \times EF_{SO_2})_{Diesel} + (RT \times Idle_{hr} \times EF_{SO_2})_{Gasoline}} \quad (2)$$

where,
$X_{SO2\text{-}idle}$ = Fraction of SO_2 due to diesel fuel, during idle
RT = Number of round trips per activity
$Idle_{hr}$ = Number of hours per trip of idle time
EF_{SO2} = SO_2 emission factor; 0.745 g/hr diesel and 0.426 g/hr gasoline.

$$X_{SO_2-run} = \frac{RT \times mi \times EF_{HDDT} + RT \times mi \times EF_{LDDT}}{T \times mi \times EF_{HDDT} + RT \times mi \times EF_{LDDT} + RT \times mi \times EF_{LDGT}} \quad (3)$$

where,
$X_{SO2\text{-}idle}$ = Fraction of SO_2 due to diesel fuel, during running
RT = Number of round trips per activity
mi = Number of miles per trip
EF_{HDDT} = SO_2 emission factor (speed dependent) for a heavy-duty diesel truck
EF_{LDDT} = SO_2 emission factor (speed dependent) for a light-duty diesel truck
EF_{LDGT} = SO_2 emission factor (speed dependent) for a light-duty gasoline truck.

The vehicle types, miles per trip, and speeds were presented in Table 3 of EPA (2011). The EPA report also contains vehicle SO_2 emission factors by speed.

GHG emissions (CO_2, N_2O, and CH_4) were estimated using emission factors from GREET (Argonne, 2011) and EPA's AP-42 (2011). The GREET emission factors were slightly higher than the AP-42 emission factors as seen in Table 1.

Table 1. GHG emission factors.

	Diesel low (g/MJ)	Diesel high (g/MJ)	Gas low (g/MJ)	Gas low (g/MJ)
CO_2	71.70	73.36	66.21	71.70
CH_4	0.001694	0.001694	0.004922	0.004922
N_2O	0.0008598	0.0008598	0.002275	0.002275

For each activity, GHG emissions were estimated using the following equation:

$$EF_{GHG-activity} = FuelConsumption \times \rho_{fuel} \times LHV_{fuel} \times EF_{GHG} \quad (4)$$

where,
$EF_{GHG\text{-}activity}$ = Emission factor for the activity, g/activity
Fuel Consumption = Fuel consumption, liters of diesel or gasoline
ρ = Fuel density, 0.832 kg/l diesel and 0.7197 kg/l gasoline
LHV = lower heating value, 35.80 MJ/l diesel and 34.66 MJ/l gasoline
EF_{GHG} = GHG emission factor for the activity, g/MJ (see Table 1).

Tables 2-4 summarize the emission factors by activity. Table 2 shows the lower end of the range of completion/recompletion activities, and Table 3 shows the upper end of the range. A

more comprehensive summary of the emission factors and the spreadsheets used to develop these factors have been uploaded to the project wiki, http://wiki.icse.utah.edu/Wiki.jsp?page=Main.

Table 2. Criteria pollutant emission factors by activity.

	SO_x	Nox	CO	VOC	PM_{10}	PM2.5
	ton/spud	ton/spud	ton/spud	ton/spud	ton/spud	ton/spud
Drilling						
Pad construction	1.32E-04	6.25E-03	2.47E-03	8.32E-04	3.94E-04	3.83E-04
Pipe construction	1.60E-04	7.14E-03	2.81E-03	1.27E-03	5.42E-04	5.26E-04
Construction traffic	3.26E-06	8.11E-04	9.08E-06	2.19E-04	4.49E-03	5.31E-04
Drilling traffic	1.26E-04	3.18E-02	1.56E-02	7.01E-03	1.34E-01	1.68E-02
Completion/recompletion						
Completion traffic	2.15E-04	5.53E-02	2.46E-02	9.81E-03	1.99E-01	2.38E-02
Recompletion traffic	4.19E-07	9.55E-05	3.45E-07	1.21E-05	7.24E-04	9.13E-05
Rework						
Refracking	2.54E-04	1.33E-02	2.28E-05	1.69E-03	5.78E-04	5.61E-04
Fracking	3.07E-03	1.21E-01	2.46E-02	1.19E-02	4.55E-03	4.42E-03
	ton/well	ton/well	ton/well	ton/well	ton/well	ton/well
Production						
Maintenance	1.19E-03	5.67E-02	2.58E-04	8.73E-03	3.16E-03	3.07E-03
Ancillary equipment	2.44E-04	1.58E-02	5.19E-03	2.33E-03	1.67E-03	1.62E-03
Production traffic	4.77E-06	1.19E-03	2.93E-05	4.52E-04	8.44E-03	9.21E-04
Maintenance traffic	1.43E-06	3.59E-04	2.37E-03	8.83E-05	1.68E-03	2.11E-04
Commuter traffic	2.80E-05	4.19E-03	5.56E-03	1.75E-03	1.73E+00	4.10E-01
Ancillary traffic	2.12E-06	4.20E-05	9.97E-04	5.03E-05	3.38E-03	3.39E-04

Table 3. Maximum emission factors for recompletion traffic.

Activity	SO_x	Nox	CO	VOC	PM10	PM2.5	Diesel	Gasoline
	ton/spud	ton/spud	ton/spud	ton/spud	ton/spud	ton/spud	ton/spud	ton/spud
Recompletion traffic	1.039-05	0.002368	2.570E-05	0.0002993	0.017963	0.002265	0.004905	0.003278

Table 4. Fuel consumption and GHG emission factors by activity.

	Diesel	Gasoline	CO_2 min	CH_4 min	N_2O min	$CO_{2\ max}$	CH_4 max	N_2O max
Activity	ton/spud	ton/spud	ton/spud	ton/spud	ton/spud	ton/spud	ton/spud	ton/spud
Drilling								
Pad construction	8.58E-02	0.00E+00	2.65E-01	6.25E-06	3.18E-06	3.07E-05	1.21E-09	5.79E-10
Pipe construction	1.04E-01	0.00E+00	3.21E-01	7.59E-06	3.86E-06	3.73E-05	9.76E-10	7.03E-10
Construction traffic	1.05E-03	1.88E-03	9.24E-03	7.68E-08	2.45E-07	1.09E-06	5.60E-12	2.96E-11
Drilling traffic	7.00E-02	2.08E-02	2.82E-01	5.10E-06	4.87E-06	3.29E-05	3.72E-10	7.22E-10
Completion/recompletion								
Completion traffic	1.32E-01	1.48E-02	4.53E-01	9.59E-06	6.49E-06	5.27E-05	6.99E-10	1.07E-09
Recompletion traffic	1.98E-04	1.32E-04	1.03E-03	1.44E-08	2.18E-08	1.21E-07	1.05E-12	2.92E-12
Rework								
Refracking	1.66E-01	0.00E+00	5.11E-01	1.21E-05	6.13E-06	5.93E-05	8.80E-10	1.12E-09
Fracking	2.01E+00	0.00E+00	6.19E+00	1.46E-04	7.42E-05	7.18E-04	1.07E-08	1.35E-08
	ton/well	ton/well	ton/well	ton/well	ton/well	ton/well	ton/well	ton/well
Production								
Maintenance	7.77E-01	0.00E+00	2.40E+00	5.66E-05	2.87E-05	2.78E-04	5.28E-09	5.24E-09
Ancillary equipment	1.59E-01	0.00E+00	4.91E-01	1.16E-05	5.89E-06	5.69E-05	1.21E-09	1.07E-09
Production traffic	2.29E-03	1.43E-03	1.16E-02	1.68E-07	2.42E-07	1.36E-06	1.48E-11	3.27E-11
Maintenance traffic	4.92E-04	7.68E-04	3.97E-03	6.13E-07	1.02E-07	2.29E-06	7.92E-11	3.39E-11
Commuter traffic	8.28E-03	1.74E-02	8.11E-02	6.04E-07	2.22E-06	9.55E-06	4.40E-11	2.65E-10
Ancillary traffic	0.00E+00	2.41E-03	7.69E-03	2.86E-06	2.64E-07	9.94E-06	3.33E-10	1.35E-10

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

The project team has been delayed in completing final milestones and deliverables on this task for two reasons. First, the CFD code being used for the simulations, ARCHES, has proven to be unstable at long simulation times for all scoping cases that have been run for the burner/furnace geometry in the IFRF's oxy-gas experiments (Coraggio and Laiola, 2009). A steady state solution is needed for V/UQ, so this instability has been a significant stumbling block. There are

no stability problems for cases run with oxy-coal flames and for cases with similar boundary conditions(hot furnace walls), so it is unclear what is causing this instability. Coding changes, including the way boundary conditions are applied, are being pursued. If this problem cannot be resolved soon, the project team will use Star CCM+ in order to complete this project. The disadvantage of Star CCM+ is that radiative heat loss cannot be properly accounted for in the reaction model, which is a source of error in a strongly radiating flame like an oxy-gas flame.

Second, the student working on the project is focusing on one of the parameters to be used in the V/UQ study, the reaction/mixing model, until the CFD code problems are resolved. Currently, the only type of reaction/mixing model fully implemented in ARCHES is equilibrium chemistry with an assumed PDF of the mixture fraction to account for subgrid scale heterogeneity. The resulting state space variables (temperature, density, species mass fractions, etc.) are functions of three independent variables: mixture fraction, heat loss (scaled enthalpy) and variance of the assumed PDF distribution. This work focuses on developing a second type of reaction model, a flamelets model, that has an additional independent variable, the scalar dissipation rate χ, that can be thought of as an extent of reaction variable. With this addition, flame chemistry that is far from equilibrium can be tracked. It is thought that this type of model could have a strong impact on the output variables of interest in an oxy-gas system such as local CO_2 and NO_x concentrations and heat release (e.g. radiative heat transfer). A summary of the algorithm the student has proposed to generate the tables needed for this new reaction/mixing model is attached as Appendix B.

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

The milestone to develop preliminary modules in $CLEAR_{uff}$ for conventional oil & gas development in the Uinta Basin was completed in this quarter. ProMax models for both on-site treatment of raw natural gas and of produced water were also developed and will be implemented into the $CLEAR_{uff}$ framework in the next quarter. Lastly, data mining from well completion reports and production data from DOGM for Uinta Basin oil and gas wells continued. The information gathered is summarized in on online database at http://wiki.icse.utah.edu/Wiki.jsp?page=Data%20Collection%20from%20the%20DOGM%20well%20files.

The new production process module, OilProduction, includes the main production phases for oil and gas. The main inputs to the oil/gas production module, including drilling schedule, well depth distributions, production phase duration distributions, and well production curves, were obtained from the DOGM database of oil wells drilled after 2002 in the Uinta Basin. The module does not yet incorporate yet the data inputs that have been gathered from well completion reports.

Initial validation of the production module was performed with both the monthly production and cumulative production outputs. Figure 1 compares the production module output to production numbers from the DOGM database.

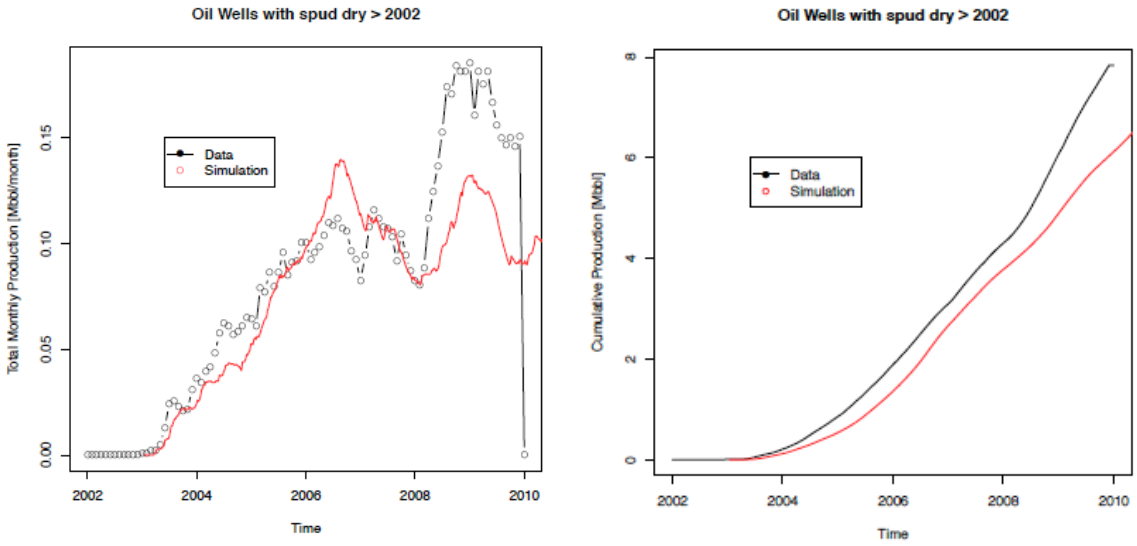


Figure 1: Comparison of simulation and DOGM data for monthly (left) and cumulative (right) production of oil wells drilled in the Uinta Basin since 2002.

Additionally, a model for the on-site treatment of raw natural gas has been developed using ProMax during this quarter. The on-site treatment of raw natural gas separates low molecular weight gases which ultimately (after further processing to remove H_2O, CO_2, N_2, NH_3 and H_2S) becomes pipeline quality natural gas, hydrocarbon liquids (natural gas condensates) and produced water. The natural gas condensates are trucked from a gas well (or a group of gas wells) to a gathering plant where they are held for sale. The produced water is mainly reinjected into the deposit to further stimulate natural gas production. In 2007, there was 550 million gallons per year of produced water in the Uinta Basin's gas wells and 14% was in excess of that which was injected (Vanden Berg, 2008). To remove particulates, produced water is treated using hydrocyclones, flotation and sand bed filtration at an on-site treatment facility. Produced water is then trucked from a gas well (or a group of gas wells) to a central gathering plant. In some cases, it is chemically treated to get it ready for reinjection and in other cases it is not. The gathered water is then trucked to the injection well where it is pumped down hole. This water can also be used for fracking operations. The model provides a mass and energy balance for the on-site process as well as the needed utilities, typically only electricity. As an Excel spreadsheet attachment to the process simulation, Subtask 3.3 researchers have developed capital and operating costs for the on-site treatment plant.

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

The milestone to develop a first generation methodology for doing V/UQ analysis was completed in this quarter. This methodology leverages work that is being done in other simulation projects within ICSE. The differences between this assessment tool and other ICSE simulation projects include both the number of parameters and the cost of a function evaluation. With the other simulation projects, one function evaluation (e.g. running the model for one set of parameters) requires several days of simulation time on a machine with 1000+ processors. Because of this expense, the size of the parameter space that can be studied is very small, i.e. on the order of 3-4 parameters, and a surrogate model must be created that can be evaluated much more cheaply. The creation of the surrogate model then becomes of critical importance to the analysis. However, with the $CLEAR_{uff}$ tool, function evaluations require something on the order of minutes on a single-processor computer. As a result, the parameter space that can be probed is much larger and the need for a surrogate model is questionable as the original model

may be fast enough to be evaluated directly.

The methodology to be applied to this system employs the Data Collaboration (DC) method proposed by Frenklach and coworkers (Feeley et al., 2004). In this paper, DC is applied to the analysis of a kinetic mechanism for natural gas combustion known as GRI-Mech. There are 650 total parameters in this system including reaction rate constants and their associated activation energies, species thermodynamic and transport properties, and instrumental constants. Function evaluations are cheap, requiring on the order of seconds. Hence, this reaction mechanism system is similar is size and run time to the $CLEAR_{uff}$ tool.

The methodology includes the following steps:

1. Determination of output variables of interest - These are the variables that will be used for validation and uncertainty quantification. Simulation outputs for these variables will be compared to experimental data. Hence, experimental data needs to be of high quality (well-resolved, uncertainties known or easily estimated). For the Uinta Basin analysis, the output variables of interest include total production rates (see Subtask 3.3), emissions of criteria pollutants (see Subtask 3.1), royalties and taxes collected, and gross domestic product (GDP).
2. Determination of active variables - In any given experiment, only a small subset of model parameters have a measurable influence on the output variable(s) of interest. These parameters are known as the active parameters (Feely et al., 2004). In the case of GRI-Mech, only 102 of the 650 parameters are active. For the $CLEAR_{uff}$ tool, the research team will need to determine the active parameter space once the modules are linked together on the platform of choice. This space will be probed based on prior experience and scoping tests.
3. Evaluation of linkage required between DCToolbox (the Matlab code available from Frenklach that includes the tools needed to perform DC) and $CLEAR_{uff}$ tool - In order to eliminate the need for the creation of a surrogate model, researchers must be able to couple DCToolbox directly with $CLEAR_{uff}$. Work is ongoing to understand whether this linkage is possible. A teleconference with Frenklach and coworkers is being held in early February 2012 to determine the best path forward. If a direct linkage is not possible, a surrogate model will be needed. The surrogate model will bound the desired parameter space and will use linear interpolation between points that are $CLEAR_{uff}$ model outputs. Previous work with quadratic interpolants shows that non-physical results can be obtained, so linear interpolants are more reliable.
4. Consistency analysis of the $CLEAR_{uff}$ output with the Uinta Basin data identified in step 1 using DCToolbox - A consistency analysis determines whether or not, given the uncertainty in the experimental data and the simulation outputs, the simulation and experimental data are consistent and over what range of parameter space this consistency occurs. If the two types of data are inconsistent, then the various parameters/models need to be reevaluated (and possibly replaced) and the error in the experimental data needs to be reanalyzed (and possibly increased).

Prior to application of the V/UQ methodology, the $CLEAR_{uff}$ framework must be modified to include all modules needed to simulate the effects of oil and gas production on regional economic and environmental conditions. In this quarter, a library of modules was collected and modifications were made to some of the modules to incorporate data/models specific to oil and gas production. Those modules include various economic sectors, GHG emissions, and population. Currently, the platform for all these modules is AnyLogic. However, due to the cost of AnyLogic licenses, the project team is investigating other platforms that might be used.

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

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

The Subtask 4.1 team has completed a topical report that details the heat transfer process inside the representative computational geometry. The report will be submitted to DOE in early February 2012.

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

The Subtask 4.1 team is using the commercial software Star-CCM+ to develop a high-performance computing (HPC), computational fluid dynamics (CFD)-based simulation tool to study thermal heating of oil shale inside the ECOSHALE capsule developed by the team's industrial partner, Red Leaf Resources. In this quarter, the team continued to improve the computational representation of the rubblized oil shale bed geometry inside the ECOSHALE capsule and to assess new features of Star-CCM+ that will hopefully eliminate the need for secondary software tools to generate rubblized oil shale bed geometries.

In previous quarterly reports, the research team has detailed the geometry creation procedure used to approximate the rubblized pieces of oil shale inside the computational domain. This procedure uses DEM simulation capabilities in Star-CCM+ to create the representative fractured pieces of shale; see Figure 2. The DEM simulation gives the location of each piece of oil shale in a Cartesian coordinate system that can be converted to a .csv file. Using Matlab for file conversion, this information is then imported into Gambit, a commercially-available software toolbox, to generate the rubblized shale bed geometry. Once the geometry is finalized in Gambit, it is exported into a parasolid format that is imported back into Star-CCM+ for the study of thermal heating process.

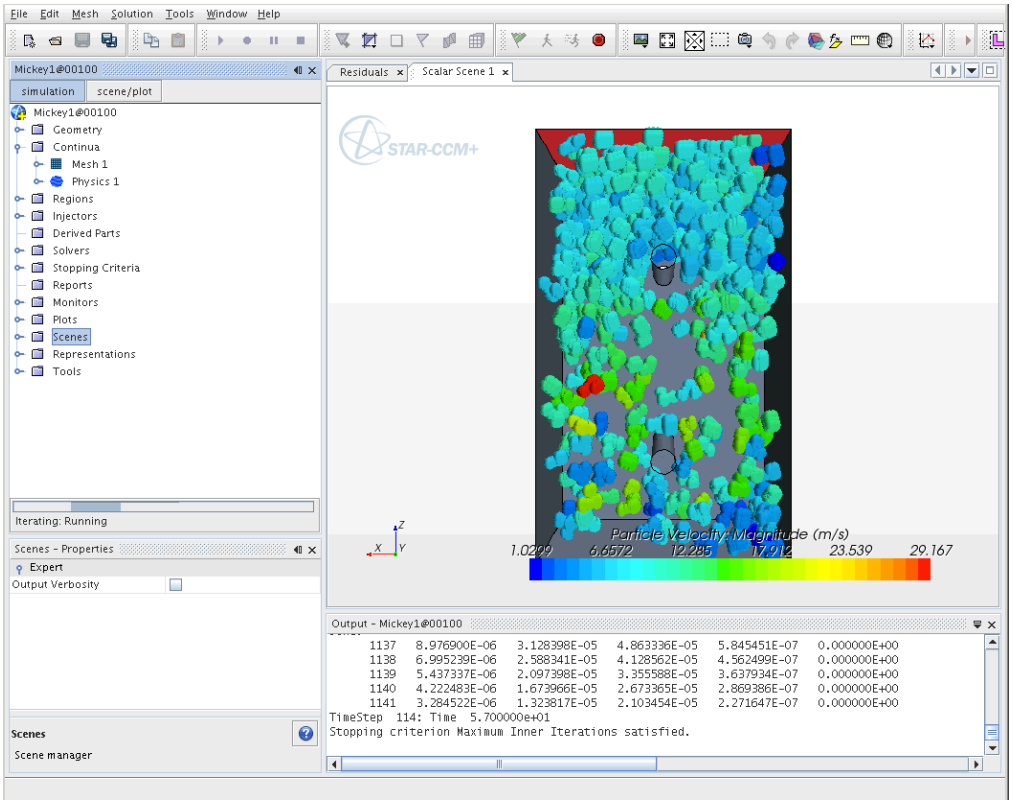


Figure 2: Star-CCM+ DEM simulation of a representative computational domain being filled with oil shale particles.

A new update with Star-CCM+ software has improved its capabilities such that it is no longer necessary to employ a separate software package. The research team is redeveloping its procedure to create simulation geometries with as few format transitions as possible. Once completed, the procedure will be less prone to error, allowing faster turn around time between geometry creation and simulation results.

Subtask 4.1 researchers continue to use the simplified geometric representation of the individual shale particles because of the meshing and the trapped internal volumes issues described in previous quarterly reports. Previously, Star-CCM+ memory limitations were reached with two particle sizes inside the computational domain. In this quarter, the complexity of the geometric representation has been increased by building on research experience with two adjacent contacting solid particles. The notion of two contacting particles was used to produce particle sizes seen in Figure 3. The particle on the right represents intersections of two oil shale particles of differing size - a larger cuboid particle and two smaller particles. Therefore, the final geometrical representation consists of particles with three distinct sizes. The research team has implemented this new geometry-generating technique with no errors and will continue to improve upon this methodology to increase the accuracy of the rubblized oil shale bed representation for the CFD simulations.

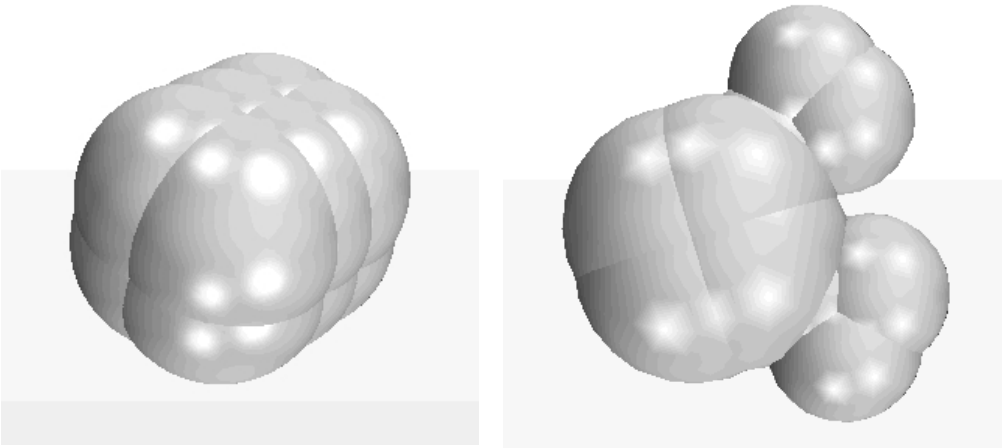


Figure 3: DEM representations of oil shale particles simulating three different sizes.

Subtask 4.1 researchers are also working to decrease the size of the convective channels between pieces of oil shale as seen in the geometric representation of the computational domain in Figure 4. These improvements will increase the accuracy of the CFD simulations.

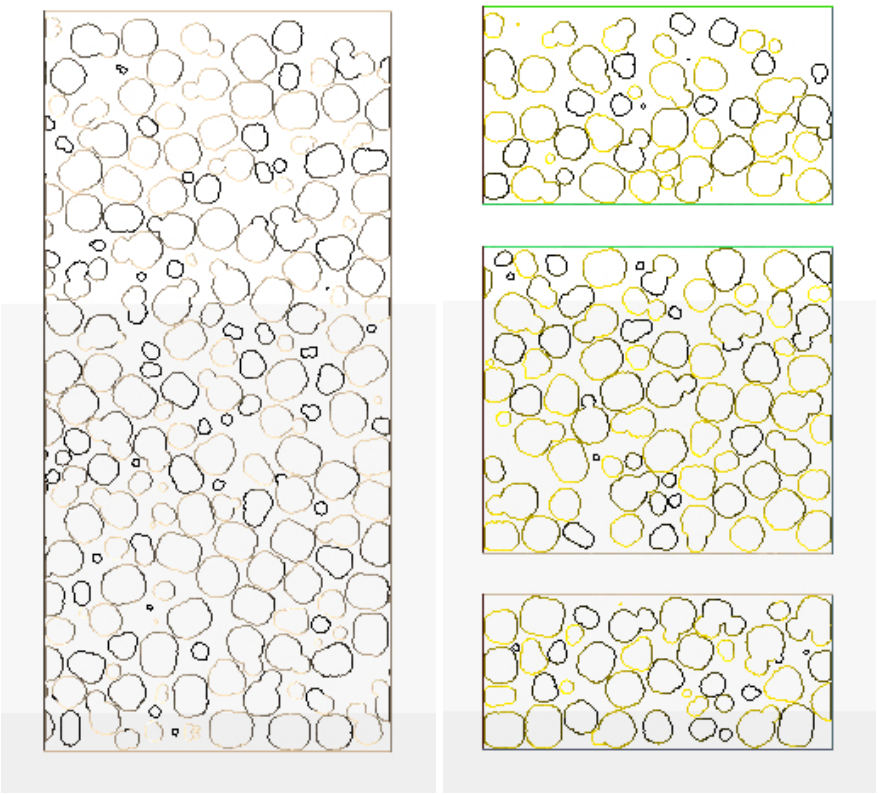


Figure 4: Improved geometric representation for the simulation domain containing oil shale pieces of three different sizes with decreased sizes of convective heating channels between the pieces of oil shale. (left) Front view. (right) Side view showing upper and lower heating pipes.

Finally, the Subtask 4.1 continues to improve the operator splitting algorithm. As it was developed, this algorithm requires user input to switch from the small fluid time-scale mode to the large thermal time-scale mode. Efforts in this quarter were in the direction of automating the algorithm with a completion date sometime in the next quarter.

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

The milestone to incorporate advanced kinetic and composition models for oil shale pyrolysis into commercial and new compositional reservoir simulators was completed in this quarter. STARS is a commercial compositional and thermal reservoir simulator developed by Computer Modeling Group (CMG). Within this simulator, a multi step mechanism for kerogen decomposition due to pyrolysis has been used to study various in situ oil shale pyrolysis processes. The mechanism essentially accounts for the cracking of long hydrocarbon chains at pyrolysis temperatures. The model is relatively simple to maintain computational efficiency while appreciating some of the major compositional effects on reservoir behavior. In the equations below, HO = Heavy Oil and LO = Light Oil.

$$\text{Kerogen} \rightarrow \text{HO} + \text{LO} + \text{Gas} + CH_4 + \text{Char}$$

$$\text{HO} \rightarrow \text{LO} + \text{Gas} + CH_4 + \text{Char}$$

$$\text{LO} \rightarrow \text{Gas} + CH_4 + \text{Char}$$

$$\text{Gas} \rightarrow CH_4 + \text{Char}$$

$$\text{Char} \rightarrow CH_4 + \text{Gas} + \text{Coke}$$

Experiments show that the kinetics for kerogen pyrolysis reactions depend on the time and the temperature history of the heated samples. One way to account for the differences in pyrolysis rates due to different heating rates is to represent kerogen decomposition with a distribution of activation energies. In STARS, kerogen is represented by seven components with different activation energies according to the following distribution shown in Figure 5.

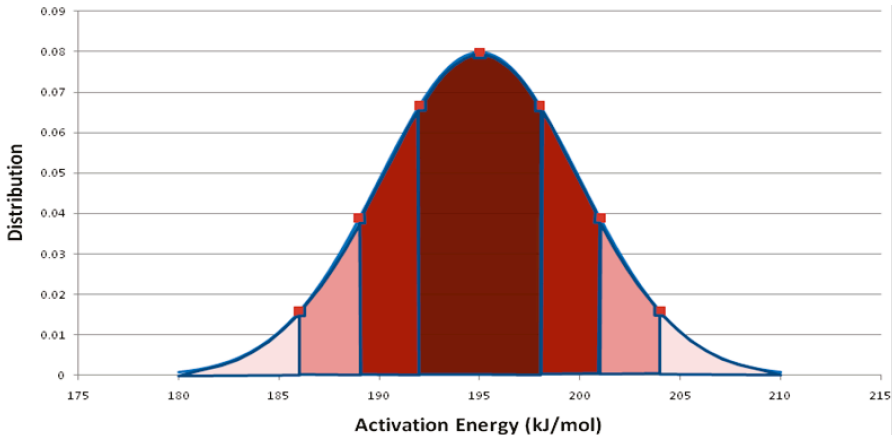


Figure 5: Distribution of activation energies for components used to represent kerogen.

The multistep oil shale pyrolysis mechanism was also incorporated into COMSOL multiphysics software. COMSOL is a finite element package that couples many physical models and solves them simultaneously. Heat transfer, chemical kinetics, and fluid flow models are solved in COMSOL to explore the behavior of fluid compositions obtained from oil shale samples with different time and temperature histories. Figure 6 shows COMSOL simulation results for the product composition obtained from 10-cm oil shale core pyrolysis experiments.

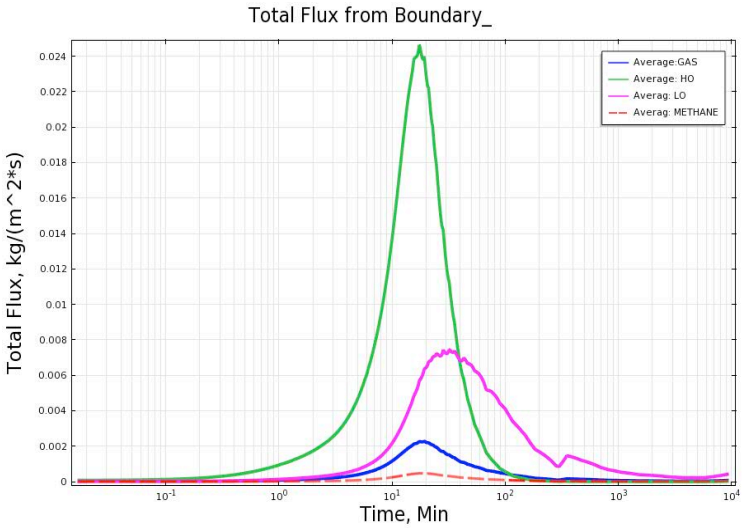


Figure 6: Mass fluxes of various oil and gas streams obtained from a COMSOL simulation of an oil shale core pyrolysis experiment.

Finally, a model for representing kerogen pyrolysis with a distribution of activation energies dependent on kerogen conversion has been incorporated into the Advanced Reactive Transport Simulator (ARTS) at the University of Utah. Results will be discussed in future quarterly reports.

In other work, Subtask 4.2 researchers have focused on some of the major challenges with in situ oil shale development in the U.S.: energy efficiency, energy input required for heating, and CO_2 emissions from the heating energy source, gas flaring, carbonate mineral decomposition, etc. These challenges make oil shale a less competitive source of liquid fuel, despite the vast local resources. A possibility for addressing some of these issues is the sequential combination of in situ pyrolysis, in situ combustion, and CO_2 EOR. Based on previous simulation results, in situ pyrolysis alone requires a large energy input and makes the process either prohibitively slow because of reliance on conductive heating or the number of wells that must be drilled excessive because of small spacing between wells. Past experiences with in situ combustion field testing have shown that it is difficult to generate sufficient initial permeability and to control combustion. Also, a portion of the producible resource is consumed for the purpose of fueling the process.

During in situ pyrolysis, it is believed that permeable pathways should develop. Cracking kerogen to liquids and vapors will leave behind some coke and other residual organic material that cannot be produced. After a period of time, pyrolysis should generate adequate permeability and coke to begin in situ combustion by air injection. In situ combustion heats the reservoir more efficiently with a moving heat boundary and does not require any external heat generation. The process then fuels itself. After a period of in situ combustion, a period of CO_2 injection for EOR and for CO_2 storage then takes place. Figure 7 shows that pyrolysis generates permeability and coke near the heaters such that in situ combustion can begin.

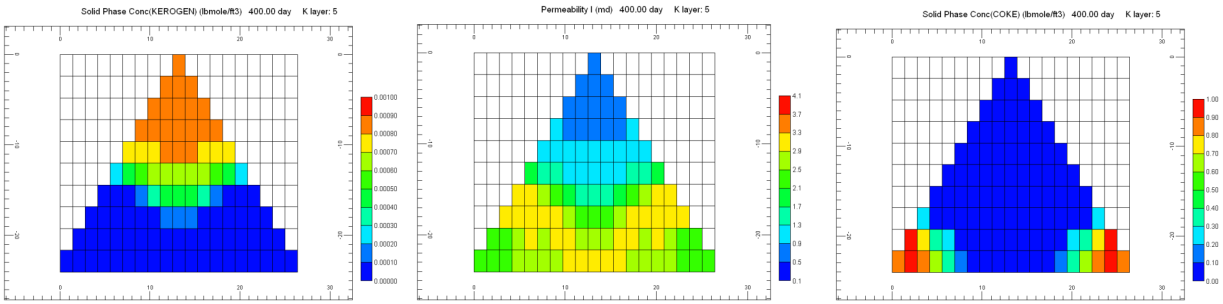


Figure 7: (left) Kerogen concentration, (middle) horizontal permeability, and (right) coke concentration after 400 days of in situ pyrolysis heating.

One of the parameters for optimizing this combined strategy is the time for switching from in situ pyrolysis to in situ combustion. Figures 8 and 9 show, as a function of time, the energy supplied by heaters during pyrolysis and the cumulative oil production for switching times of 100, 400, 600, and 800 days. With this geometry, the optimal switching time is between 100 and 400 days since the cumulative production is essentially constant for switching times of ≥400 days. The CO_2 reinjection step did not store much CO_2 or produce significantly more oil with the modeling parameters used in these simulations.

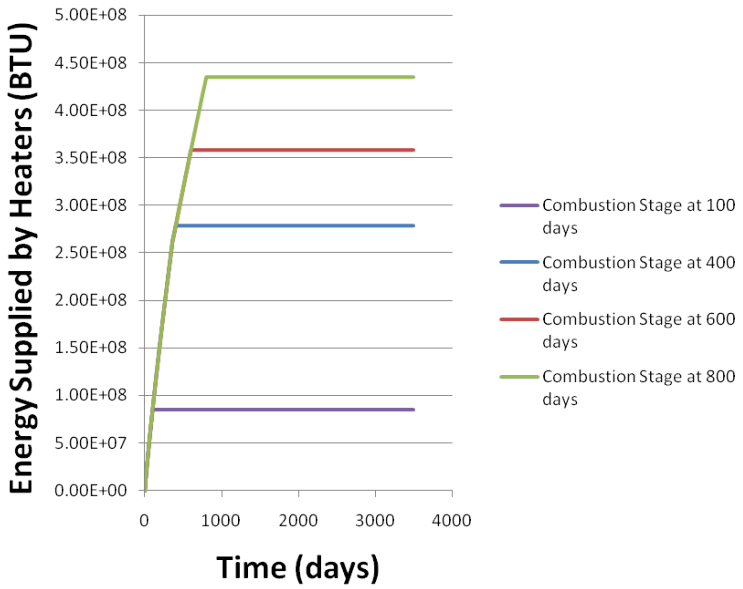


Figure 8: Cumulative energy input where pyrolysis is switched to in situ combustion at different times.

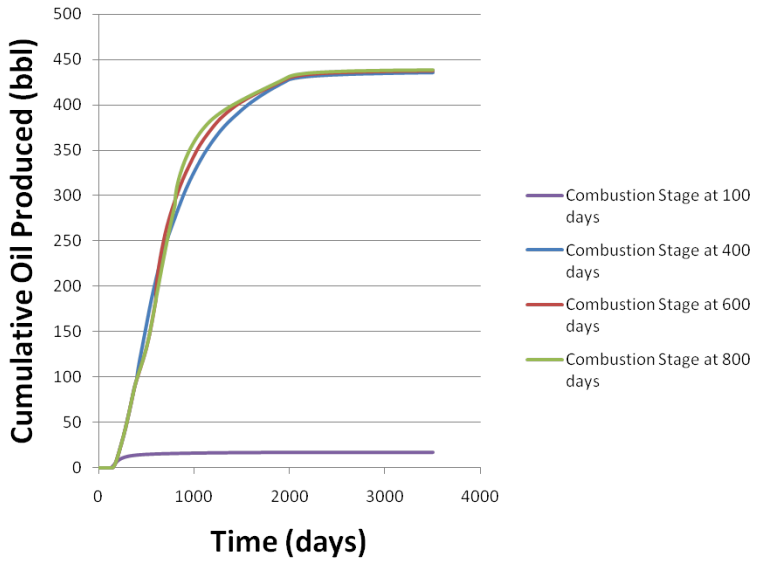


Figure 9: Cumulative oil production where pyrolysis is switched to in situ combustion at different times.

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

The milestone to complete core sample pyrolysis at various pressures and to analyze product bulk properties and composition was not completed in this quarter. This delay is due to the heterogeneity of the three oil shale core samples described next. Because of this heterogeneity, the samples were divided into three pieces each and additional testing was performed, delaying the planned completions of experiments at pressure.

For the work described in this report, three fresh, organic-rich (Mahogany zone) samples from the Skyline 16 core were selected. These samples are GR-1 (461.9- 462.9 feet), GR-2 (485.9-486.9 feet) and GR-3 (548.1- 549.1 feet).

In a previous quarterly report, the Subtask 4.3 team summarized the TGA and the carbon, hydrogen, nitrogen, and sulfur (CHNS) elemental analysis data on homogeneous powdered samples of GR-1, GR-2 and GR-3. Significant variation was found in terms of organic and elemental composition in these samples. Cores of 1" diameter and ~6" long samples from GR-1, GR-2 and GR-3 sections were divided into three sections each and pyrolyzed in a reactor; pyrolysis products were collected. The results of isothermal pyrolysis for 24 hours of these nine core samples were described in last quarter's report.

This report summarizes TGA pyrolysis of kerogen extracted from oil shale. The kerogen from homogenous powdered samples of GR-1, GR-2 and GR-3 sections was extracted in the Chemistry Department at the University of Utah using a series of strong acids (demineralization process). All TGA experiments were performed at a heating rate of 10˚C/min up to 1000˚C in a nitrogen environment. The spent materials were subsequently combusted from 400˚C to 600˚C (10˚C/min) and held for 10 minutes at 600˚C without opening the furnace chamber in order to quantify coke production. An overlaid thermogram of these three runs is shown in Figure 10. The results from the TGA analysis are summarized in Table 5. The results show that for all three kerogens, onset points (start and end) in the pyrolysis zone were close to identical. The onset points of kerogen (extracted) decomposition also coincide with the organic matter onset points of oil shale under the identical conditions (Figure 11). The kerogen (extracted) weight losses

differ with the difference in the final weight loss dependent on the extent of demineralization achieved. The coke formed during pyrolysis ranged from 10-15 % of initial weight and was relatively higher for GR-1. The TGA of GR-1oil shale also showed higher coke than GR-2 and GR-3 oil shale; see the quarterly report from July 2011.

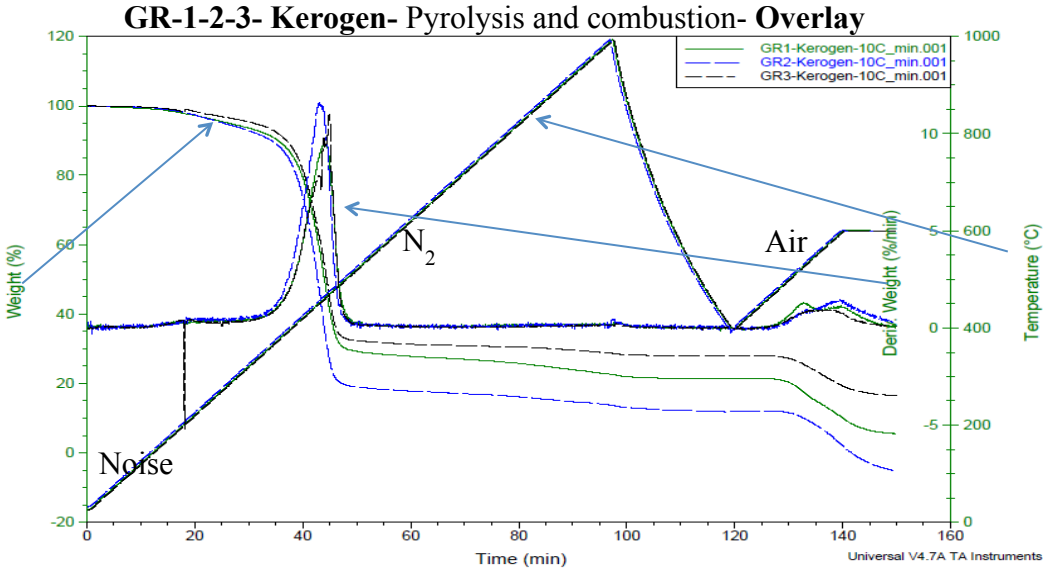


Figure 10: Pyrolysis followed by combustion of three powdered kerogens extracted from GR-1, GR-2 and GR-3 samples.

Table 5. Summary of TGA data from kerogen pyrolysis followed by combustion.

Samples	Initial mass, mg	Py-end T	Py- wt loss %	Com- wt loss %	Final- wt loss %
GR1-Kerogen-10°C_min	4.32	514°C	70.58	15.57	94.32
GR2-Kerogen-10°C_min	2.30	513°C	80.81	11.98	103.12
GR3-Kerogen-10°C_min	6.77	515°C	67.58	10.92	83.09

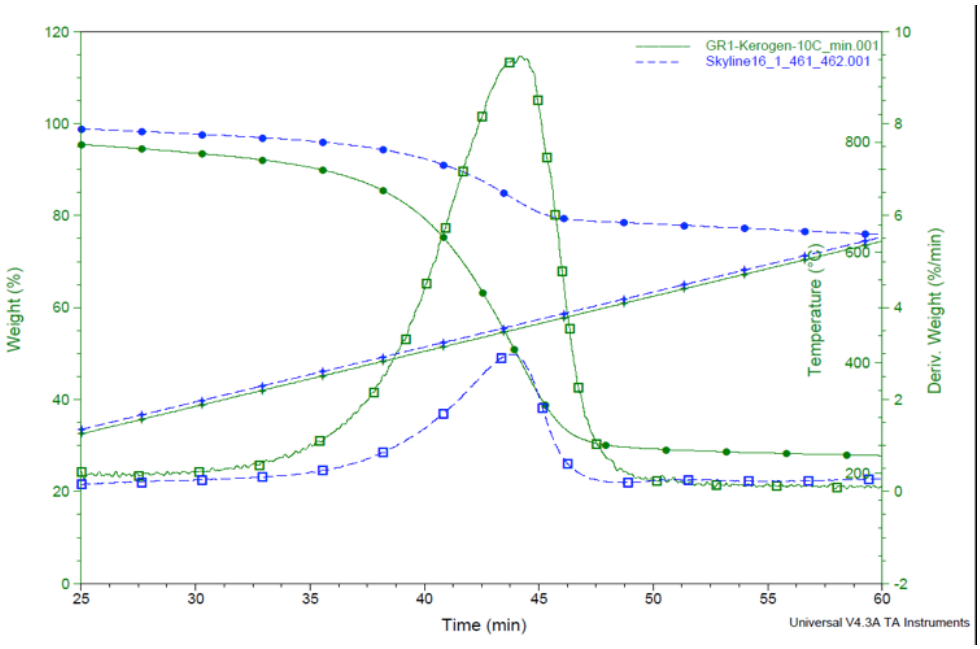


Figure 11: Comparison of the organic matter decomposition onset points during the pyrolysis of isolated kerogen (extracted) and original raw oil shale from the same source (GR-1).

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

This project has been completed.

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

Research on pore scale transport processes in the pyrolysis of oil sand and oil shale involves 3D multiscale X-ray CT analysis coupled with Lattice Boltzmann (LB) simulation. During this quarter, Subtask 4.5 researchers continued worked with three fresh Skyline 16 oil shale cores (6” long, 1” in diameter) provided by Subtask 4.3: GR-1, GR-2, and GR-3.

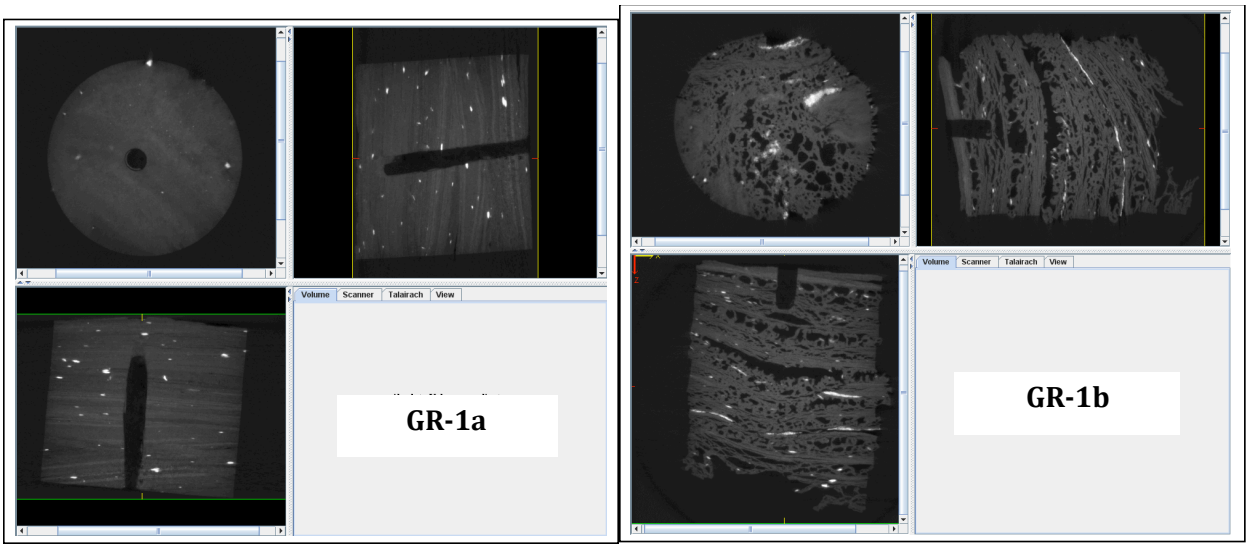
The full-length cores were scanned in sections before pyrolysis and the results reported in last quarter’s report. To investigate the effect of reaction temperature, each core was cut into three sections (2” long, 1” in diameter) and then pyrolyzed at different temperatures as described above in Subtask 4.3; the conditions are summarized in Table 6. After pyrolysis, selected pieces of these nine samples were scanned.

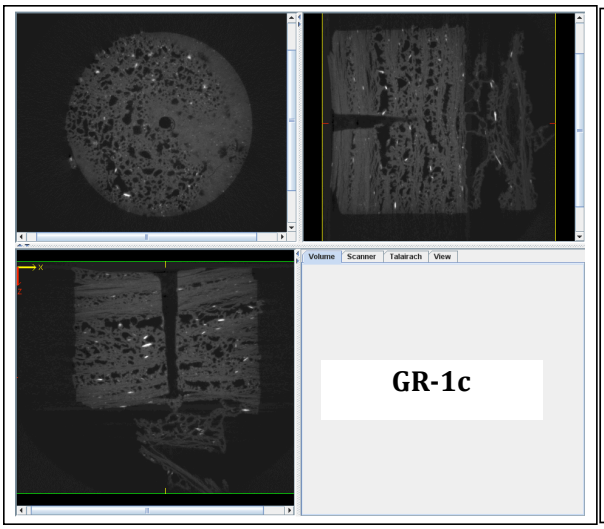
Table 6. Experimental conditions for pyrolyzed oil shale sample.

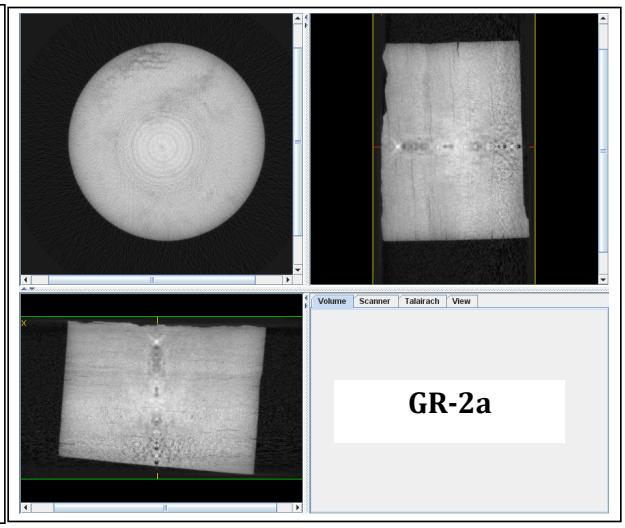
Sample No.	Initial Weight (g)	Reaction Temperature (°C)	Drill Hole Position for Thermocouple Wire
GR-1a	40.3217	350	Top
GR-1b	40.4917	425	Bottom
GR-1c	41.6266	500	Bottom
GR-2a	61.8151	425	Top

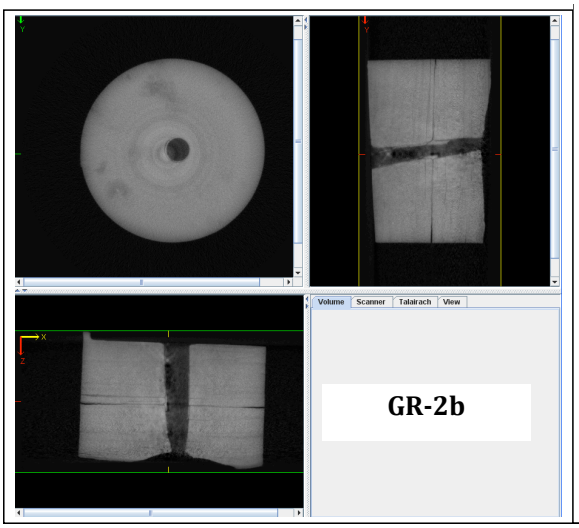
GR-2b	52.9283	500	Top
GR-2c	50.7762	325	Top
GR-3a	51.1995	500	Top
GR-3b	51.7524	350	Top
GR-3c	47.8818	425	Bottom

The tri-planar images from the reconstructed X-ray CT data (~42 micron voxel resolution) for the nine Skyline 16 oil shale drill core samples after pyrolysis (selected large chunks of these nine cores) are shown in Figure 12. As expected, pores were generated along the kerogen-rich layers, specifically for GR-1b and GR-1c samples. Directional fractures along the thin, kerogen-rich layers are observed for GR-2 and GR-3 samples. Characterization of the texture change during pyrolysis is in progress by comparing the same sections of cores before and after pyrolysis.




Volume
Scanner
Talairach
View
GR-1c


Volume
Scanner
Talairach
View
GR-2a


Volume
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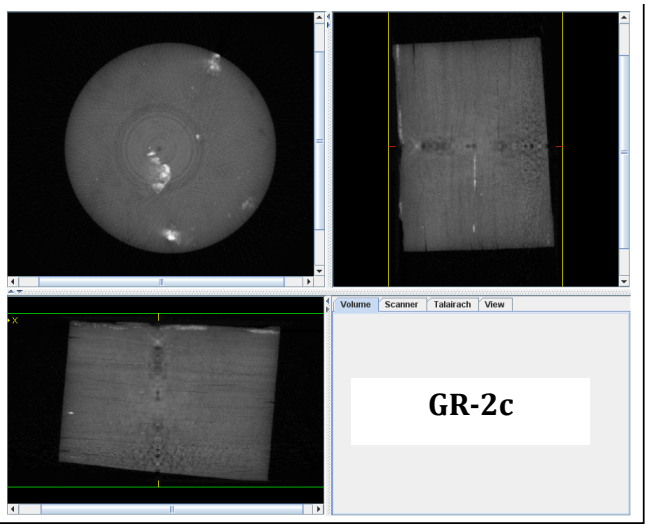
GR-2b


Volume
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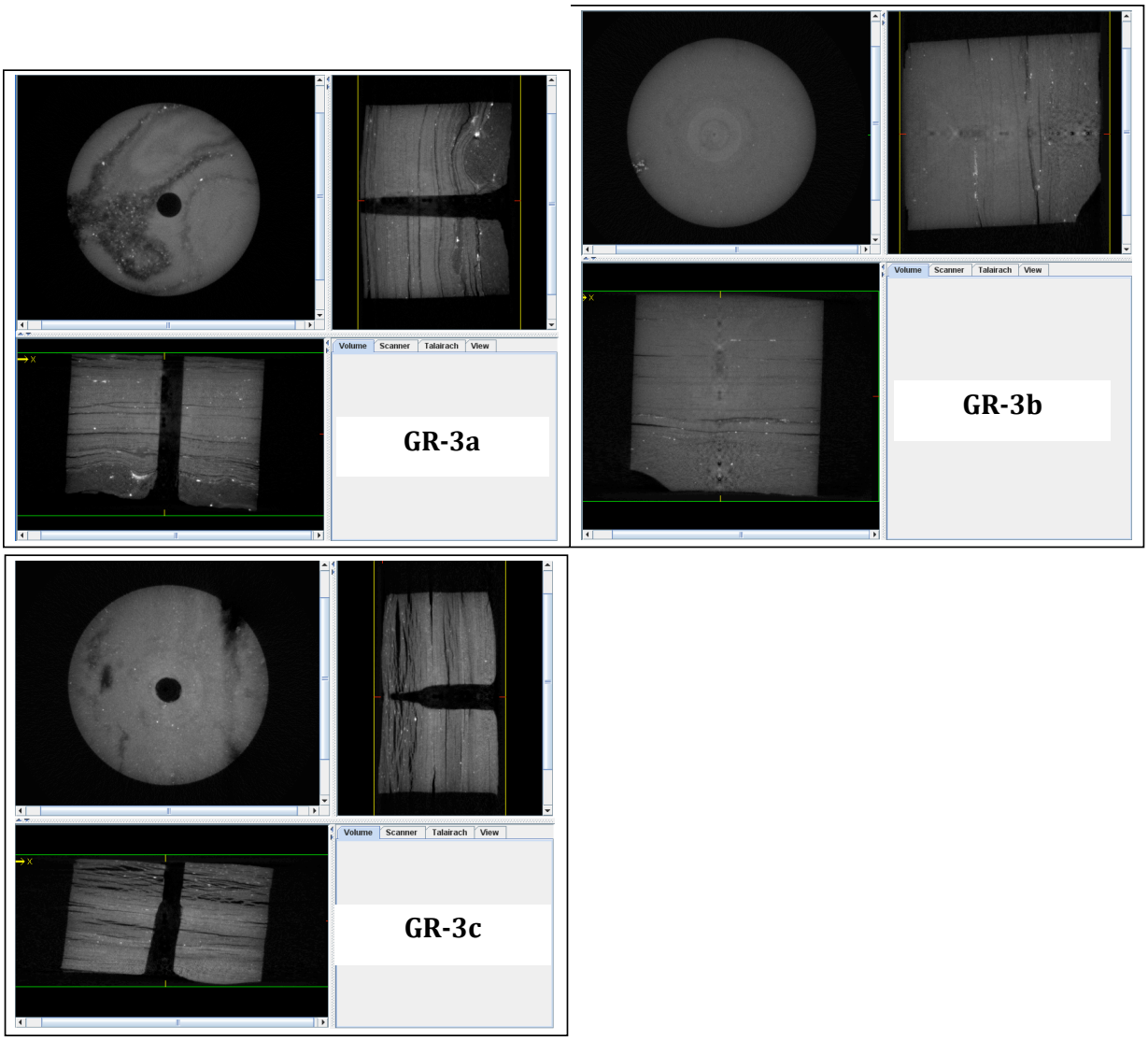

Figure 12: Tri-planar images from reconstructed X-ray CT data (~42 micron voxel resolution) for nine Skyline 16 oil shale drill core samples after pyrolysis.

The research team will next investigate directional (anisotropic) permeability of the nine pyrolyzed samples based on pore network structure by X-ray CT analysis coupled with LB simulation.

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

In this quarter, the milestone to create a web-based repository for both the 3D models and the calculated data for the kerogens, asphaltenes, and complete systems was completed. The repository currently contains the asphaltene models (as both figures and pdb atomic coordinate files) and the calculated nuclear magnetic resonance (NMR) data based on these models. The kerogen models along with their calculated observables will be added when the kerogen paper is submitted. The link to the repository is: http://www.oilshalesands.utah.edu/index.jsp?leftnavid=3;&page=27

Most of the time in this quarter was spent on completing two manuscripts. The asphaltene manuscript was submitted and the kerogen manuscript is in final draft form; see the "Presentation/Publication" section of this report.

To complete the asphaltene paper, Subtask 4.6 researchers explored how changing the 2D model affects the simulated ^{13}C solid state (SS) NMR spectrum. To do this, an alternate model for the Mid-Continent US asphaltene was built – one with the same aromatic core but with the aliphatic carbon content divided among the substituent locations. This model still fits all of the criteria upon which the original model was based. The new model, shown as both the 2D and 3D structures in Figure 13, was optimized and the ^{13}C SSNMR was calculated (Figure 14). As can be seen from this figure, the peak intensity of the aliphatic region and the general shape of the aliphatic region in the spectrum from the alternate model (mc-2) are in better agreement with the experimental spectrum than the original model (mc).

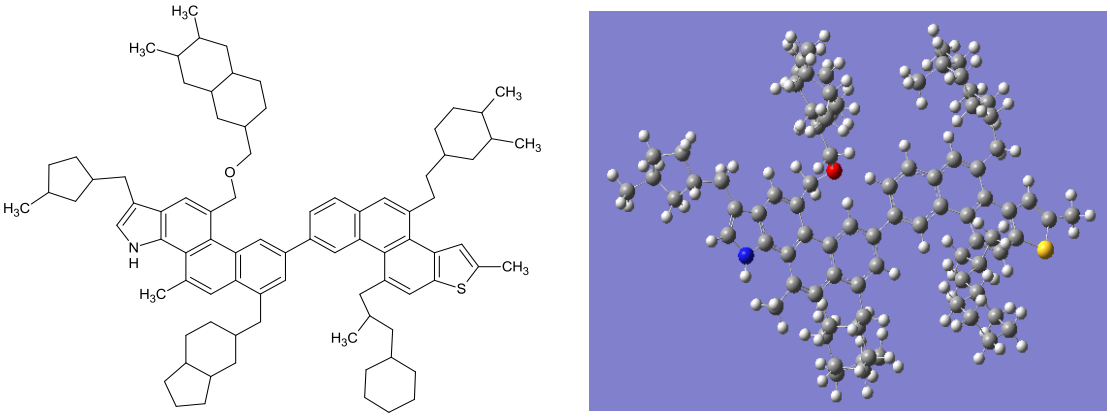

Figure 13: Alternate model, shown both as 2D and 3D, for Mid-Continent US asphaltene.

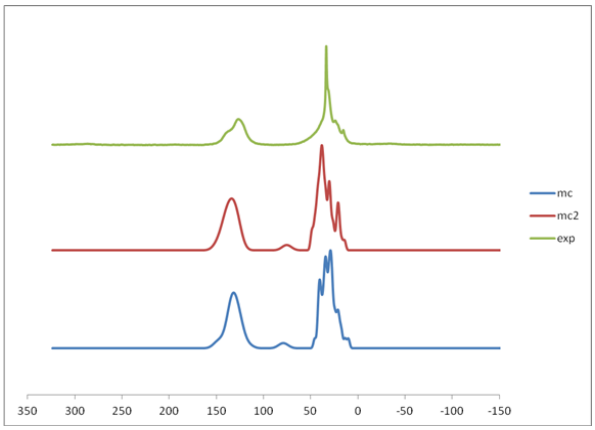

Figure 14: ^{13}C SSNMR spectra for the alternate Mid-Continent US asphaltene (mc-2) compared with both the experimental spectrum (Siskin et al., 2006) and the equivalent spectrum obtained using the original model (mc).

To study the effect of the interaction of organic materials with inorganic materials on the NMR spectrum, team members performed NMR shielding calculations on the previously modeled mc asphaltene-illite system, shown in Figure 15. These results are compared with the spectrum of a

single mc-asphaltene and with experimental data in Figure 16. From this figure, it is clear that there are changes in the spectrum, especially in the aromatic region.

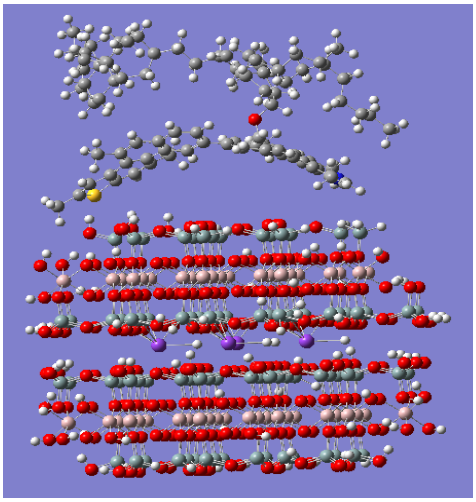

Figure 15: Model of interaction between Mid-Continent US asphaltene and illite.

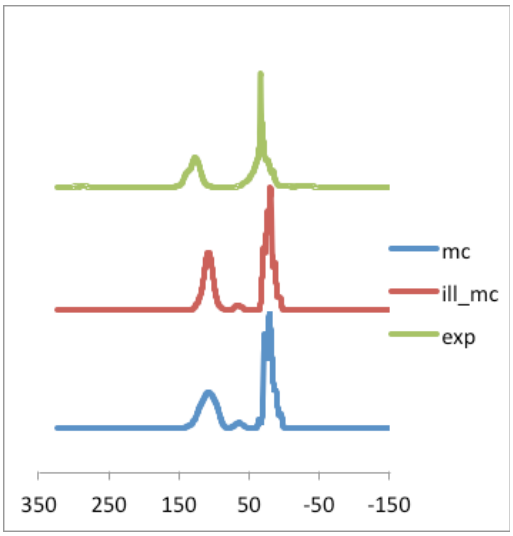

Figure 16: Comparison of the simulated ^{13}C SSNMR spectra based on the model in Figure 15 (ill_mc) with both the original model without the illite (mc) and experimental spectrum from Siskin et al. (2006).

The research team also returned to the kerogen project now that both ^{13}C SSNMR and pairwise PDF measurements have been taken on the kerogen isolated from segments of the ICSE Skyline 16 core. The experimental work was completed as part of a Subtask 4.9. ^{13}C NMR spectra were simulated based on the shielding calculations for different 3D structures that the research team previously generated based on the 2D kerogen model proposed by Siskin and Katritksy (1995). Figure 17 shows the simulated ^{13}C SSNMR spectra for five different conformations and Figure 18 shows the comparison between the experimental and the simulated spectra based on the lowest energy conformation.

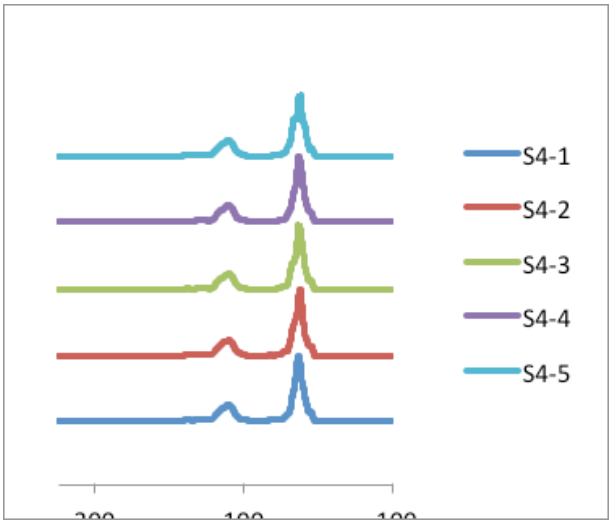

Figure 17: Simulated ^{13}C NMR spectra for kerogen models S4-1 through S4-5.

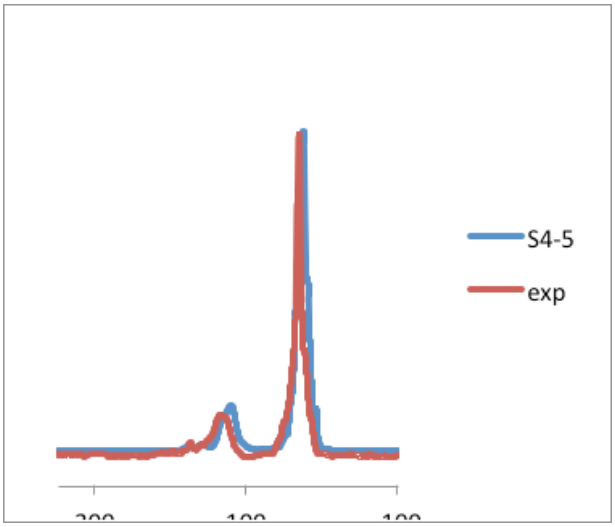

Figure 18: Comparison between simulated ^{13}C NMR spectrum from model S4-5 and the experimental solid state ^{13}C NMR spectrum obtained from kerogen isolated from a segment of the ICSE Skyline 16 core.

As part of subtask 4.9, a PDF measurement was also made on the kerogen. Figure 19 shows a comparison between the PDF simulated based on the dodecamer kerogen model and the experimental PDF plot.

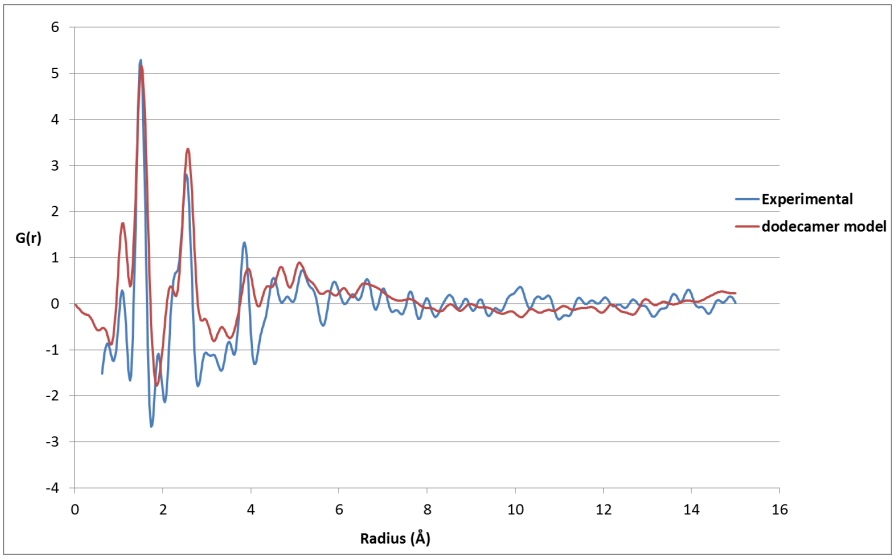

Figure 19: Comparison of the experimentally-determined PDF obtained from the kerogen isolated from a segment of the ICSE Skyline 16 core and the simulated PDF based on the dodecamer version of the ICSE 3D kerogen model.

Dr. Anita Orendt is visiting the Advanced Photon Source (APS) at Argonne National Laboratory in February 2012 to obtain more experimental data (both SAXS and PDF measurements) as part of Subtask 4.9 and to coordinate on the further evaluation of the ICSE kerogen model with collaborators at the facility.

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

During this quarter, the project team continued an accumulation and evaluation of available literature describing the thermal properties and mechanical properties of oil shales, predominantly based on public domain literature from the western U.S. Team members also continued the accumulation of components for the experimental apparatus for the in-situ testing of Skyline 16 core samples. There has also been a substantial redesign of the internal fixtures, allowing for additional stability and ease of access to the sample; see Figure 20. The project team is currently designing the system for safely and effectively evaluating the produced liquids and gases in conjunction with Subtask 4.3 researchers.

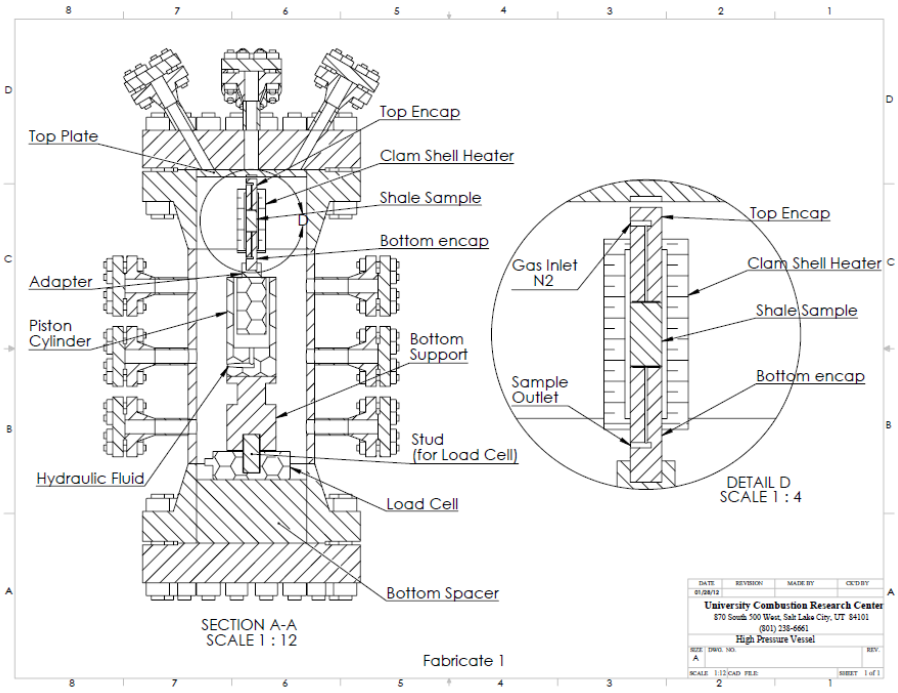

Figure 20: Schematic of the pressure vessel to be used for in-situ testing of oil shale core samples.

Team members have been consulting with staff in Civil Engineering about the design of the internal measurement systems, specifically the measurement of axial and radial deformation of the samples while they are being tested. The project team anticipates a continued collaboration with Civil Engineering to do an ambient temperature dry run of the internal instrumentation and sample stack – outside of the pressure vessel – using one of the large testing frames used for structural engineering testing.

Samples that have been tested in the apparatus are being sent to a third party testing facility for determination of permeability and porosity.

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

The PI for this project is on maternity leave, so no research was conducted during this quarter.

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

Last quarter, Subtask 4.9 researchers reported that additional acid washes were needed to obtain demineralized kerogen samples. Kerogen samples now exist for each of the three previously identified segments from the ICSE Skyline 16 core (GR-1, GR-2, and GR-3); ashing tests confirm that the mineral content of each of these samples is approximately 5%. Samples have been provided to researchers in Subtasks 4.3 and 4.5 for pyrolysis experiments, X-ray CT analysis, and TGA analysis. Additional samples have been set aside for a February 2012 trip to the APS at Argonne National Laboratory for SAXS and additional PDF measurements. Along with the kerogen, the bitumen extracts were also isolated for solution NMR analysis.

Solid state ^{13}C CPMAS and SPMAS NMR studies were completed on the GR-3 kerogen to add to the data previously reported for the GR-1 and GR-2 kerogens and the shales of all three; all spectra are shown in Figure 21. The SPMAS and CPMAS spectra of the kerogens are, within the S/N differences, identical; for the shales, the single pulse spectra show the presence of the inorganic carbonates.

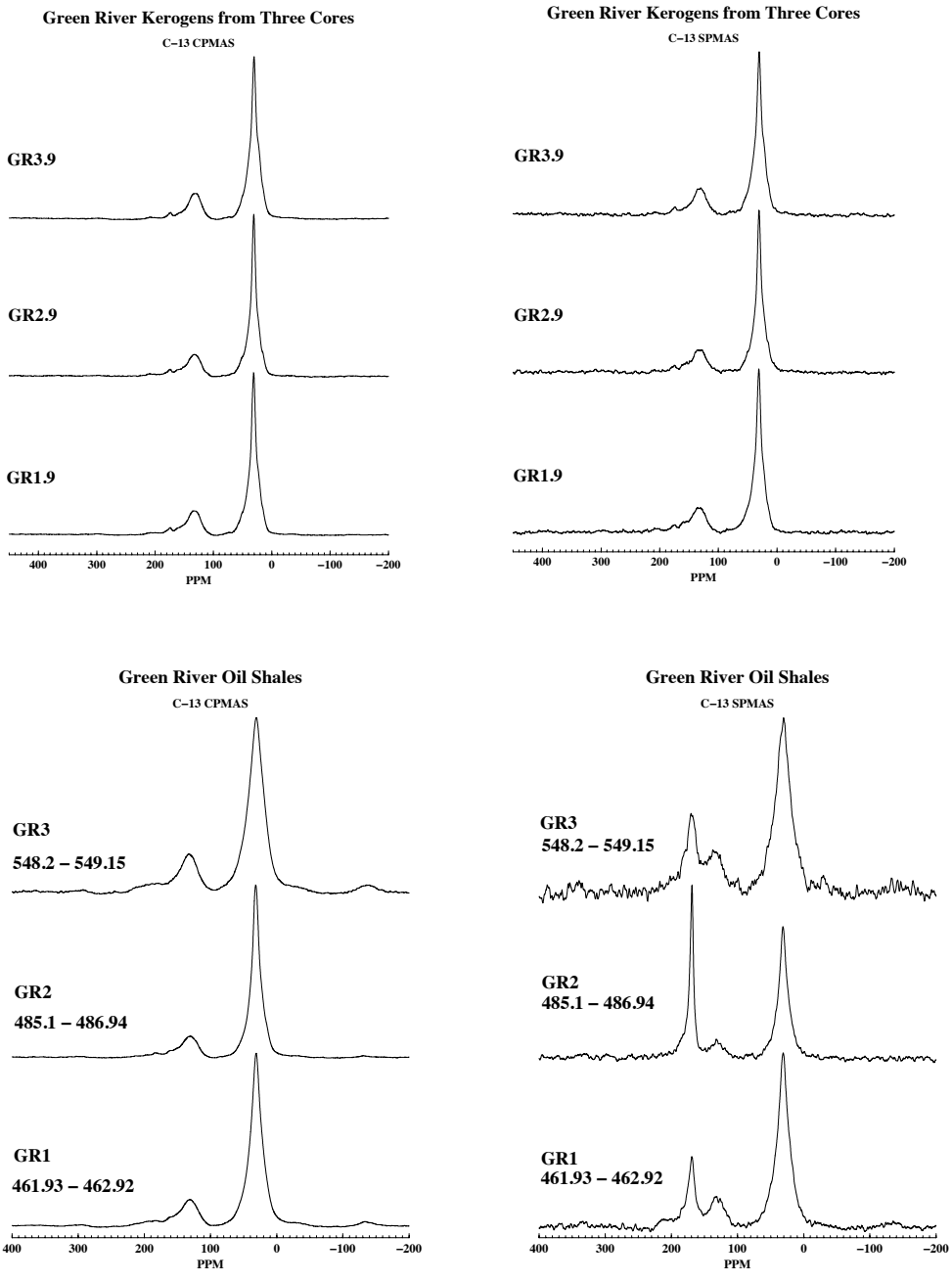

Figure 21: *Top, left*: The CPMAS spectra of the three kerogens taken with a 3 ms contact time. There is no peak at about -130 ppm showing that ferromagnetic minerals have been removed during demineralization. *Top, right*: The SPMAS spectra of the three kerogens taken with a 30 s pulse delay. *Bottom, left*: CPMAS spectra of the three shales taken with a 3 ms contact time.

Notice the peak at -130 ppm in GR1 and GR3 due to ferrimagnetic minerals. *Bottom, right*: SPMAS spectra of the three shales taken with a 30 s pulse delay. The sharp peak at about 174 ppm is due to inorganic carbonates not seen in CPMAS spectra.

The structural and lattice parameters extracted from the CPMAS spectra are given in Table 6 for both the shales and kerogens. The previously reported data for the shale GR-3 was reevaluated due to larger than expected spinning sidebands from the aliphatic material overlapping the sp^2 region of the spectra. Spinning sidebands are usually not seen for aliphatic material due to the small chemical shift anisotropy of these carbons, unless they arise due to ferromagnetic or ferrimagnetic material in the sample changing magnetic fields as the sample spins. The aromaticity of the kerogens determined via a single pulse experiment is also included in Table 6.

As can be seen from the data in Table 7, the organic matter is very similar for the three kerogens. The aromaticity, 0.27, is highest in GR-3.9 and lowest, 0.22, in GR-2.9. This difference is just slightly larger than the errors in the measurement. There is no significant change in structure during demineralization and extraction of the bitumen, as seen by a comparison of the shale and kerogen results from each segment. All the samples have an average aromatic cluster size of about 10 ± 2 carbons, corresponding to average clusters approximately the size of naphthalene. The samples are highly crossed linked to the aromatic centers with the lattice coordination number, σ + 1, having values between 4.4 and 6.0.

Along with the ^{13}C solid state NMR on the kerogen, solution ^{13}C NMR was also completed on the bitumen extracted from the GR-2 segment. The spectra obtained include a quantitative ^{13}C spectrum to provide accurate determination of the amount of different carbon types and a DEPT series to identify carbons in terms of the number of attached protons. Attempts at doing 2D heteronuclear correlation experiments to get further information about molecular structure failed due to inadequate resolution and poor signal to noise due to limited solubility. Obtaining similar data on the bitumen extracted from the GR-1 and GR-3 segments is planned.

From the quantitative ^{13}C NMR, shown in Figure 22, it is determined that aliphatic carbons dominate the sample, with only 6% aromatic carbons and a trace of acid and/or ester carbonyl carbons. A closer inspection of the aliphatic region, along with the use of chemical shift additivity rules, allows the average length of aliphatic chains to be estimated at approximately 24 carbons. Analysis of the DEPT spectra indicates that methylene carbons (CH_2) are the dominate type of aliphatic carbon and that there are very few methine (CH) or quartenary carbons, indicating that branching in the aliphatic chain is not common.

Finally, the project team received initial atomic PDFs taken on GR-1 and GR-2 samples by Dr. Karena Chapman of the APS in October 2011; these are shown in Figure 23. The PDF of the two kerogen samples is also nearly identical with the same pattern of peaks, even at longer atomic separations. When Dr. Orendt travels to the APS in February 2012, she will obtain the PDF from the GR-33 kerogen as well as consult with Dr. Chapman about the analysis of this data.

Table 7. Green River shales and their kerogens from three cores.

Structural Parameters														
Compound	f_a	C f_a	O f_a	OO f_a	f_a'	H f_a	N f_a	P f_a	S f_a	B f_a	f_{al}	H f_{al}	$*$ f_{al}	O f_{al}
GR-1 (CP) cr	0.25	0.04	0.02	0.02	0.21	0.07	0.14	0.04	0.07	0.03	0.75	0.62	0.13	0.02
GR-1.9 (CP)	0.24	0.04	0.01	0.03	0.20	0.06	0.14	0.03	0.07	0.04	0.76	0.65	0.11	0.00
GR-1.9 (SP)	0.25										0.75			
GR-2 (CP) nc	0.22	0.04	0.02	0.02	0.18	0.06	0.12	0.03	0.06	0.03	0.78	0.65	0.13	0.00
GR-2.9 (CP)	0.23	0.05	0.02	0.03	0.18	0.06	0.12	0.03	0.06	0.03	0.77	0.66	0.11	0.01
GR-2.9 (SP)	0.24										0.76			
GR-3 (CP) cr	0.27	0.03	0.01	0.02	0.24	0.06	0.18	0.04	0.08	0.06	0.73	0.60	0.13	0.05
GR-3.9 (CP)	0.24	0.04	0.01	0.03	0.20	0.05	0.15	0.03	0.07	0.05	0.76	0.63	0.13	0.00
GR-3.9 (SP)	0.25										0.75			

Lattice Parameters								
Compound	χ^b	C	$\sigma+1$	P 0	$B.L.$	$S.C.$	$M.W.$	$M\delta$
GR-1 (CP)	0.143	8.4	4.4	-0.18	--	--	--	--
GR-1.9 (CP)	0.200	10.0	5.0	-0.10	--	--	--	--
GR-2 (CP)	0.167	9.0	4.5	-0.44	--	--	--	--
GR-2.9 (CP)	0.167	9.0	4.5	-0.22	--	--	--	--
Gr-3 (CP)	0.250	12.0	6.0	-0.08	--	--	--	--
Gr-3.9 (CP)	0.250	12.0	5.9	-0.30	--	--	--	--

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

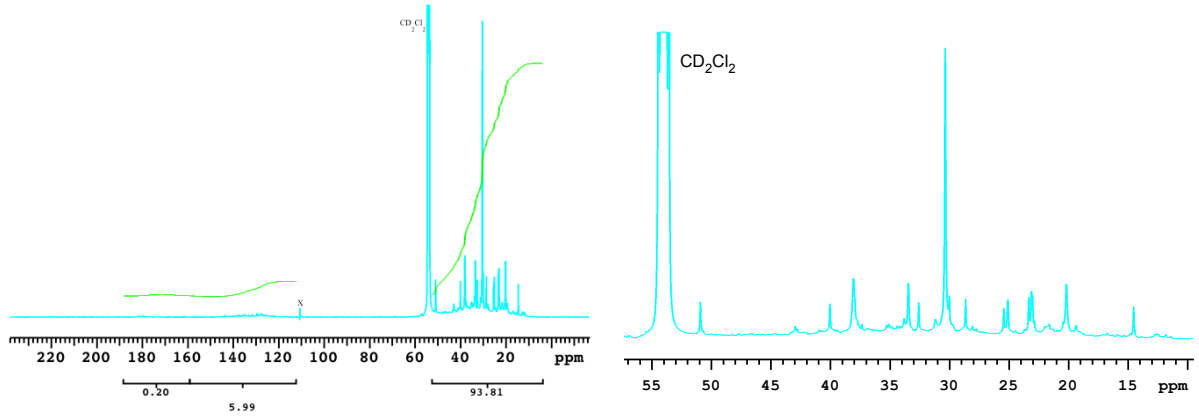

Figure 22: Quantitative (NOE suppressed) ^{13}C NMR spectrum of GR-2 bitumen dissolved in CD_2Cl_2. The X indicates a spectrometer artifact. An expansion of the aliphatic region is shown to the right.

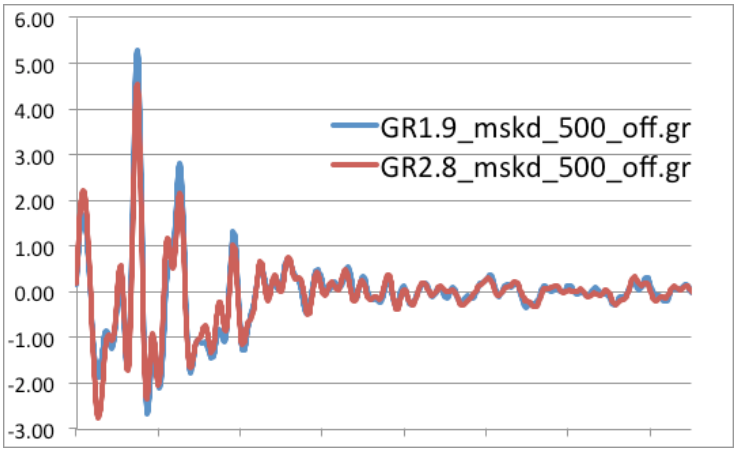

Figure 23: Atomic PDFs for the kerogen isolated from the GR-1 and GR-2 segments of the ICSE Skyline 16 core.

Task 5.0 - Environmental, Legal, Economic and Policy Framework

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

Subtask 5.1 researchers completed drafting the topical report and circulated it to external reviewers for comment. The final version of the topical report will be submitted next quarter.

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

This quarter, Subtask 5.2 researchers integrated reviewer comments and completed the topical

report for this project for final submission.

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

Work begun on this project last quarter, but mistakenly omitted from the quarterly report, was continued this quarter. Specifically, research continued on surveying the legal standards used by the judiciary to evaluate the weight and credibility of simulations as evidence in cases addressing environmental risks or harms.

6.0 – Economic and Policy Assessment of Domestic Unconventional Fuels Industry

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

Editorial work and further calculations to support the editorial work have been performed during this quarter. The milestone to provide models used & data collected to the ICSE repository and the deliverable to provide a topical report describing the process models used and a summary of parameters analyzed are both delayed until Subtask 6.3 is completed.

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

During this quarter, Subtask 6.2 researchers continued to finalize the economic analysis portions of the report. The topical report being prepared for this Subtask is again delayed due to continuing revisions and drafting required both by reviewer comments and the need for analytic consistency between the economic analysis of oil sands presented in the topical report for this Subtask and the Market Assessment report. Additional delays have been occasioned by needed updates to the policy analysis and discussion portions of the topical report. Completion of the topical report for this Subtask is expected during the next quarter.

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

After extensive consultation with Michael Hogue, an economist in ICSE, the microeconomic analysis provided as part of the Market Assessment has two measures of profitability, a Supply Price Method and a Net Present Value Method. The first method finds the minimum price of oil that would ensure profitability of the project if that price, adjusted for inflation, were to be received on each barrel of oil sold from the project. The second method evaluates the profitability of the project when the oil prices received are those of the most recent EIA oil price forecasts. All of the scenarios are being reanalyzed using this new approach. In addition, two significant bugs were found in the cost model. These bugs have been fixed and the new results reflect the changes.

The report is currently being prepared for distribution. Due to the lateness of the report, a second draft version will not be circulated. Sections 1-6 have been sent for page layout with Section 7-10 to follow in the next two weeks. Page layout is now complete on the first five sections with the exception of minor edits for typos, etc. Page layout requires one week per section, which means the remaining five sections will require five more weeks to complete.

7.0 – Strategic Alliance Reserve

The Task 7.0 project team met with an industrial collaborator, AMSO, during this quarter for the official kickoff meeting of the SAR project. The kickoff meeting was held on October 25, 20111 at the University of Utah.

Subtask 7.1 – Geomechanical Model (PI: John McLennan)

In conjunction with Subtask 4.7, available public domain testing information is being collected that represents constitutive mechanical and thermal properties of oil shale. This public information is supplemented with information that has been generated specifically by AMSO. Various variables have been identified for use in multivariate analysis of stress-strain-porosity-permeability behavior.

Team members are also been meeting with Dr. Anthony Gary, a data analysis specialist, to assess the best methodology for processing large volumes of experimental data. This methodology has application well beyond oil shale and hopefully will delineate some procedures for developing appropriate predictions of rock deformation under a number of in-situ variables.

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

No report received.

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

Subtask 7.3 researchers are developing HPC-based computational tools to simulate the heat transfer in the rubblized oil shale bed as described in Subtask 4.1. Past research at ICSE has shown that the heat transfer in the shale bed is the rate limiting process for production of oil form oil shale and that the convective heating significantly reduces the time for the shale bed to reach the oil shale production temperature in comparison to conductive heating alone. For this subtask, researchers are applying the HPC tools developed for Subtask 4.1 to the in situ heating process proposed by AMSO.

In the October 2012 kickoff meeting with AMSO representatives, team members began to gather information regarding the geometry of their process and the specific properties of shale at their test site. They also received feedback on preliminary rubblized shale geometries. Based on the feedback, researchers have constructed a rubblized shale geometry, shown in Figure 24, that is more representative of the AMSO process.

Researchers have used HPC-based tools to create a preliminary simulation of a three-day heating process. Figure 25 shows the temperature distributions in the computational domain after about 80 hours of heating. The left part of the figure shows the temperature distribution throughout the convective heating channels (the fluid region) and the right hand side of the figure shows the temperature distribution in the solid (shale) region of the computational domain. The operator-splitting algorithm was applied to take advantage of the differing conductive and convective heating time scales occurring inside this preliminary domain.

In the next quarter, Subtask 7.3 researchers plan to implement the specific shale properties provided by AMSO as well as coordinate with researchers of Subtasks 7.1 and 7.2 to improve the physical properties of shale used in the HPC simulations.

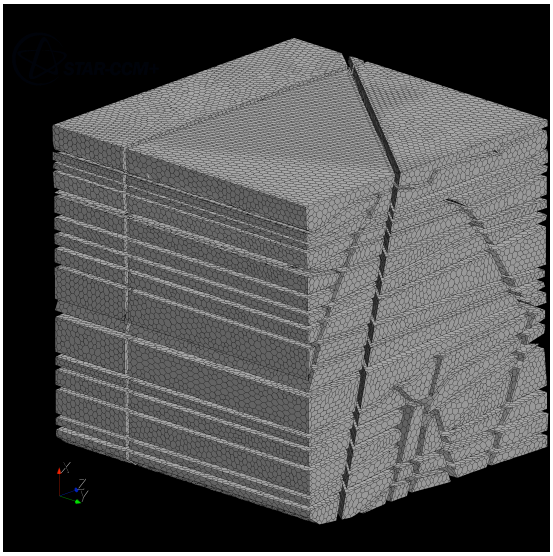

Figure 24: Preliminary rubblized shale representation of the AMSO process.

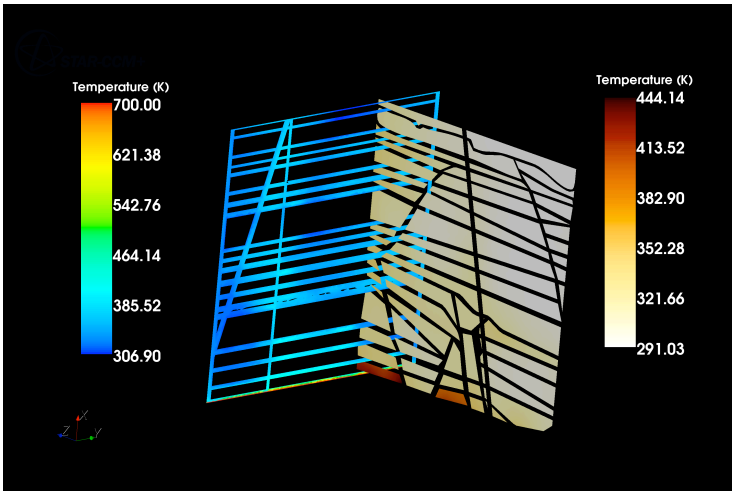

Figure 25: Temperature distribution in the preliminary computational representation of the AMSO process.

CONCLUSIONS

Two subtasks were completed during this quarter. One was Phase I of Subtask 4.1 (Development of CFD-based Simulation Tools for In-situ Thermal Processing of Oil Shale/ Sands) and the other was Subtask 5.2 (Conjunctive Management of Surface and Groundwater Resources). The topical report for Subtask 5.2 has been submitted to DOE and that for Subtask 4.1 will be submitted shortly. In addition, a project kickoff meeting with the industrial partner, AMSO, was held for Subtasks 7.1-7.3. Significant progress was made in Subtask 6.3 (Market Assessment) with the first half of the report in page layout form & ready for publishing after final proofing. The second half of the report is currently undergoing page layout. Delays in Subtask 6.3 have also led to delays in the completion of Subtasks 3.1 (Phase I), 6.1, and 6.2, so those projects will be completed in the next quarter.

COST STATUS

COST PLAN/STATUS

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

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

Baseline Reporting Quarter - PHASE II	Yr. 2				Yr. 3							
	Q7		Q8		Q9		Q10		Q11		Q12	
	04/01/11 - 06/30/11		07/01/11 - 09/30/11		10/01/11 - 12/31/11		01/1/12 - 03/31/12		04/01/12 - 06/30/12		07/01/12 - 09/30/12	
	Q7	**Total**	Q8	**Total**	Q9	**Total**	Q10	**Total**	Q11	**Total**	Q12	**Total**
Baseline Cost Plan												
Federal Share	712,385	**3,773,026**	627,423	**4,400,449**	147,451	**4,547,900**	147,451	**4,695,351**	147,451	**4,842,802**	245,447	**5,088,249**
Non-Federal Share	178,100	**943,509**	156,854	**1,100,363**	36,863	**1,137,226**	36,863	**1,174,089**	36,863	**1,210,952**	58,906	**1,269,858**
Total Planned	890,485	**4,716,535**	784,277	**5,500,812**	184,314	**5,685,126**	184,314	**5,869,440**	184,314	**6,053,754**	304,353	**6,358,107**
Actual Incurred Cost												
Federal Share	449,459	**3,078,729**	314,813	**3,393,542**	271,897	**3,665,439**		**3,665,439**		**3,665,439**		**3,665,439**
Non-Federal Share	48,902	**699,537**	48,835	**748,372**	105,695	**854,067**		**854,067**		**854,067**		**854,067**
Total Incurred Costs	498,361	**3,778,266**	363,648	**4,141,914**	377,592	**4,519,506**		**4,519,506**		**4,519,506**		**4,519,506**
Variance												
Federal Share	262,926	**694,297**	312,610	**1,006,907**	-124,446	**882,461**		**1,029,912**		**1,177,363**		**1,422,810**
Non-Federal Share	129,198	**243,972**	108,019	**351,991**	-68,832	**283,159**		**320,022**		**356,885**		**415,791**
Total Variance	392,124	**938,269**	420,629	**1,358,898**	-193,278	**1,165,620**		**1,349,934**		**1,534,248**		**1,838,601**

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

MILESTONE STATUS

ID	Title/Description	Planned Completion Date	Actual Completion Date	Milestone Status
1.0	Project Management			
2.0	Technology Transfer and Outreach			
	Advisory board meeting	Jun-12		
	Hold final project review meeting in format determined jointly by DOE/NETL and ICSE	Jun-13		
3.0	Clean Oil Shale & Oil Sands Utilization with CO2 Management			
3.1	Lifecycle greenhouse gas analysis of conventional oil & gas development in the Uinta Basin			
	Complete modules in $CLEAR_{uff}$ for life-cycle CO2 emissions from conventional oil & gas development in the Uinta Basin	Jun-12		
3.2	Flameless oxy-gas process heaters for efficient CO2 capture			
	Preliminary report detailing results of skeletal validation/uncertainty quantification analysis of oxy-gas combustion system	Oct-11		Problems with CFD code will be addressed next quarter
3.3	Development of oil & gas production modules for $CLEAR_{uff}$			
	Develop preliminary modules in $CLEAR_{uff}$ for conventional oil & gas development & produced water management in Uinta Basin	Oct-11	Dec-11	Discussed in this report
3.4	V/UQ analysis of basin scale $CLEAR_{uff}$ assessment tool			
	Develop a first generation methodology for doing V/UQ analysis	Oct-11	Nov-11	Discussed in this report
	Demonstrate full functionality (integration of all modules) of V/UQ methodology for conventional oil & gas development in Uinta Basin	Apr-12		
4.0	Liquid Fuel Production by In-Situ Thermal Processing of Oil Shale/Sands			
4.1	Development of CFD-based simulation tool for in-situ thermal processing of oil shale/ sands			

ID	Title/Description	Planned Completion Date	Actual Completion Date	Milestone Status
	Expand modeling to include reaction chemistry & study product yield as a function of operating conditions	Feb-12		
4.2	Reservoir simulation of reactive transport processes			
	Incorporate kinetic & composition models into both commercial & new reactive transport models	Dec-11	Dec-11	Discussed in this report
	Complete examination of pore-level change models & their impact on production processes in both commercial & new reactive transport models	Jun-12		
4.3	Multiscale thermal processes			
	Complete thermogravimetric analyses experiments of oil shale utilizing fresh “standard” core	Sep-11	Sep-11	Discussed in Oct. 2011 quarterly report
	Complete core sample pyrolysis at various pressures & analyze product bulk properties & composition	Dec-11		Delayed until next quarter
	Collection & chemical analysis of condensable pyrolysis products from demineralized kerogen	May-12		
	Complete model to account for heat & mass transfer effects in predicting product yields & compositions	Jun-12		
4.5	In situ pore physics			
	Complete pore network structures & permeability calculations of Skyline 16 core (directional/anisotropic, mineral zones) for various loading conditions, pyrolysis temperatures, & heating rates	Mar-12		
4.6	Atomistic modeling of oil shale kerogens & oil sand asphaltenes			
	Complete web-based repository of 3D models of Uinta Basin kerogens, asphaltenes, & complete systems (organic & inorganic materials)	Dec-11		Discussed in this report
4.7	Geomechanical reservoir state			
	Complete high-pressure, high-temperature vessel & ancillary flow system design & fabrication	Sep-11	Sep-11	Discussed in Oct. 2011 quarterly report
	Complete experimental matrix	Feb-12		
	Complete thermophysical & geomechanical property data analysis & validation	Apr-12		

ID	Title/Description	Planned Completion Date	Actual Completion Date	Milestone Status
4.8	Developing a predictive geologic model of the Green River oil shale, Uinta Basin			
	Detailed sedimentologic & stratigraphic analysis of three cores &, if time permits, a fourth core	Dec-12		
	Detailed mineralogic & geochemical analysis of same cores	Dec-12		
4.9	Experimental characterization of oil shales & kerogens			
	Characterization of bitumen and kerogen samples from standard core	Jan-12	Jan-12	Email sent to R. Vagnetti
	Development of a structural model of kerogen & bitumen	Jun-12		
5.0	Environmental, legal, economic, & policy framework			
5.1	Models for addressing cross-jurisdictional resource management			
	Identify case studies for assessment of multi-jurisdictional resource management models & evaluation of utility of models in context of oil shale & sands development	Jun-11	Jul-11	Discussed in Oct. 2011 quarterly report
5.2	Conjunctive management of surface & groundwater resources			
	Complete research on conjunctive surface water & groundwater management in Utah, gaps in its regulation, & lessons that can be learned from existing conjunctive water management programs in other states	Aug-11	Aug-11	Discussed in Oct. 2011 quarterly report
5.3	Policy & economic issues associated with using simulation to assess environmental impacts			
	White paper describing existing judicial & agency approaches for estimating error in simulation methodologies used in context of environmental risk assessment and impacts analysis	Dec-12		
6.0	Economic & policy assessment of domestic unconventional fuels industry			
6.1	Engineering process models for economic impact analysis			
	Upload all models used & data collected to repository	Oct-11		Still incomplete; discussed in the quarterly report

ID	Title/Description	Planned Completion Date	Actual Completion Date	Milestone Status
7.0	Strategic Alliance Reserve			
	Conduct initial screening of proposed Strategic Alliance applications	Mar-11	Mar-11	
	Complete review and selection of Strategic Alliance applications	Jun-11	Jul-11	Discussed in Oct. 2011 quarterly report
	Implement new Strategic Alliance research tasks	Sep-11	Sep-11	Discussed in Oct. 2011 quarterly report
7.1	Geomechanical model			
	Infer permeability-porosity-temperature relationships, develop model that can be used by other subtasks	Dec-12		
	Make experimental recommendations	Aug-13		
7.2	Kinetic compositional models & thermal reservoir simulators			
	Incorporate chemical kinetics into thermal reservoir simulators	Jun-12		
	Demonstrate reservoir simulation of AMSO process	Sep-12		
	Incorporate poroelastic & geomechanical models into reservoir simulator	Jun-13		
7.3	Rubblized bed HPC simulations			
	Collect background knowledge from AMSO about characteristics & operation of heated wells	Jun-12		
	Perform generation 1 simulation - DEM, CFD & thermal analysis of characteristic section of AMSO rubblized bed	Sep-12		
	Perform generation 2 simulation that incorporates kinetic compositional models from subtask 7.2 and/or AMSO	Jun-13		

NOTEWORTHY ACCOMPLISHMENTS

Collaborative research among Subtasks 4.3, 4.5, 4.6, 4.7, and 4.9 continues with each team performing different types of tests analyses on the same three samples from the Skyline 16 oil shale core (GR-1, GR-2, and GR-3).

PROBLEMS OR DELAYS

The topical report for Subtask 3.1 detailing results of lifecycle GHG emissions from a refinery or upgrader using conventional & oxy-fuel flameless technologies is again delayed due to the focus on completing Subtask 6.3, the Market Assessment. Also delayed are the topical reports for Subtasks 6.1 and 6.2. The Market Assessment is in the final stages of preparation, so all of these deliverables will be completed in the next quarter.

Subtask 3.2 is delayed until the PI finished the Market Assessment and can focus attention on code instabilities that are causing problems with simulations of the IFRF furnace. A Subtask 4.3 milestone is delayed due to sample heterogeneity that required additional testing for the three oil shale cores. Subtask 4.7 has experienced slight delays, particularly in fabrication of components. If this lengthy turnaround time continues, other options for machining parts are being considered.

RECENT AND UPCOMING PRESENTATIONS/PUBLICATIONS

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

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

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

Orendt, A., Facelli, J. C. & Pugmire, R. (2011, October). Atomistic modeling of oil shale kerogens and asphaltenes. Paper presented at the 31st Oil Shale Symposium, Colorado School of Mines, Golden, CO.

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

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

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

Vanden Berg, M. & Birgenheier, L. (2011, October). Not all rich zones are created equal: Geologic characterization results of Green River formation core descriptions from Utah's

Uinta Basin, including the newly drilled Skyline 16 core. Paper presented at the 31st Oil Shale Symposium, Colorado School of Mines, Golden, CO.

Tiwari, P. & Deo, M. (2011, October) Compositional and kinetic analysis of oil shale pyrolysis using TGA-MS. *Fuel*, available online, in press.

Wilkey, J. (2011, December). Evaluation of the economic feasibility of heavy oil production processes for West Sak Field. MS Thesis, University of Utah, Salt Lake City, UT.

R. Keiter, J. Ruple, H. Tanana and R. Holt. (2012, January). Conjunctive surface and groundwater management in Utah: Implications for oil shale and oil sands development. Submitted to the Department of Energy under DOE Award No. DE-FE0001243.

Tiwari, P. & Deo, M. (2012, February). Detailed kinetic analysis of oil shale pyrolysis TGA data. *AICHE Journal*, *58(2*), 505-515.

Rosenberg, M., Birgenheier, L. & Vanden Berg, M. (2012, April) Outcrop examination and sequence stratigraphy of the lacustrine Green River Formation, Uinta Basin, Utah: Implications for conventional and unconventional oil and gas development. Paper to be presented at the annual meeting of the American Association of Petroleum Geologists.

Eby, D., Chidsey, T., Vanden Berg, M. & Laine, M. (2012, April). Microbial carbonates from core and outcrop, Tertiary (Eocene) Green River Formation, Uinta Basin, Utah. Paper to be presented at the annual meeting of the American Association of Petroleum Geologists.

Badu, S., Pimienta, I. S. O., Orendt, A. M. Facelli, J. C. & Pugmire, R. J. (n.d.). Modeling of asphaltenes: Assessment of sensitivity of ^{13}C SSNMR to molecular structure. Submitted to *Energy & Fuels,* December 15, 2011.

Bauman. J. H. & Deo, M. D. (n.d.) Simulation of a conceptualized combined pyrolysis, in situ combustion, and CO_2 storage strategy for fuel production from Green River oil shale. Submitted to *Energy and Fuels*.

Pimienta, I. S. O., Orendt, A. M., Pugmire, R. J., Facelli, J. C., Locke, D. R., Winans, R. E., Chapman, K. W. & Chupas, P. J. (n.d.). Three-dimensional structure of the Siskin Green River oil shale kerogen model: A computational study. Manuscript in final draft form and will be submitted to a journal soon.

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

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Feeley, R., Seiler, P., Packard, A. & Frenklach, M. (2004). Consistency of a reaction dataset. *J. Phys. Chem. A, 108*, 9573-9583.

Siskin, M. & Katritksy, A. (1995). In C. Snape (Ed.), *Composition, Geochemistry and Conversion of Oil Shales*, NATO ASO Series, Series C: Mathematical and Physical Sciences-Vol. 455. Dordrecht/Boston/London: Kluwer Academic Publishers.

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

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U.S. Environmental Protection Agency. (2011, July). *Oil and gas mobile sources pilot study, Gasoline and diesel industrial engines*. Novato, CA: Environ International Corporation. Available from http://www.epa.gov/ttn/chief/ap42/ch03/final/c03s03.pdf.

Vanden Berg, M. D. (2008, December 9). *Water-related issues affecting conventional oil and gas recovery and potential oil shale development in the Uinta Basin*. Salt Lake City, UT: Utah Geological Survey. Available from http://geology.utah.gov/emp/UBwater_study/pdf/overview1208.pdf.

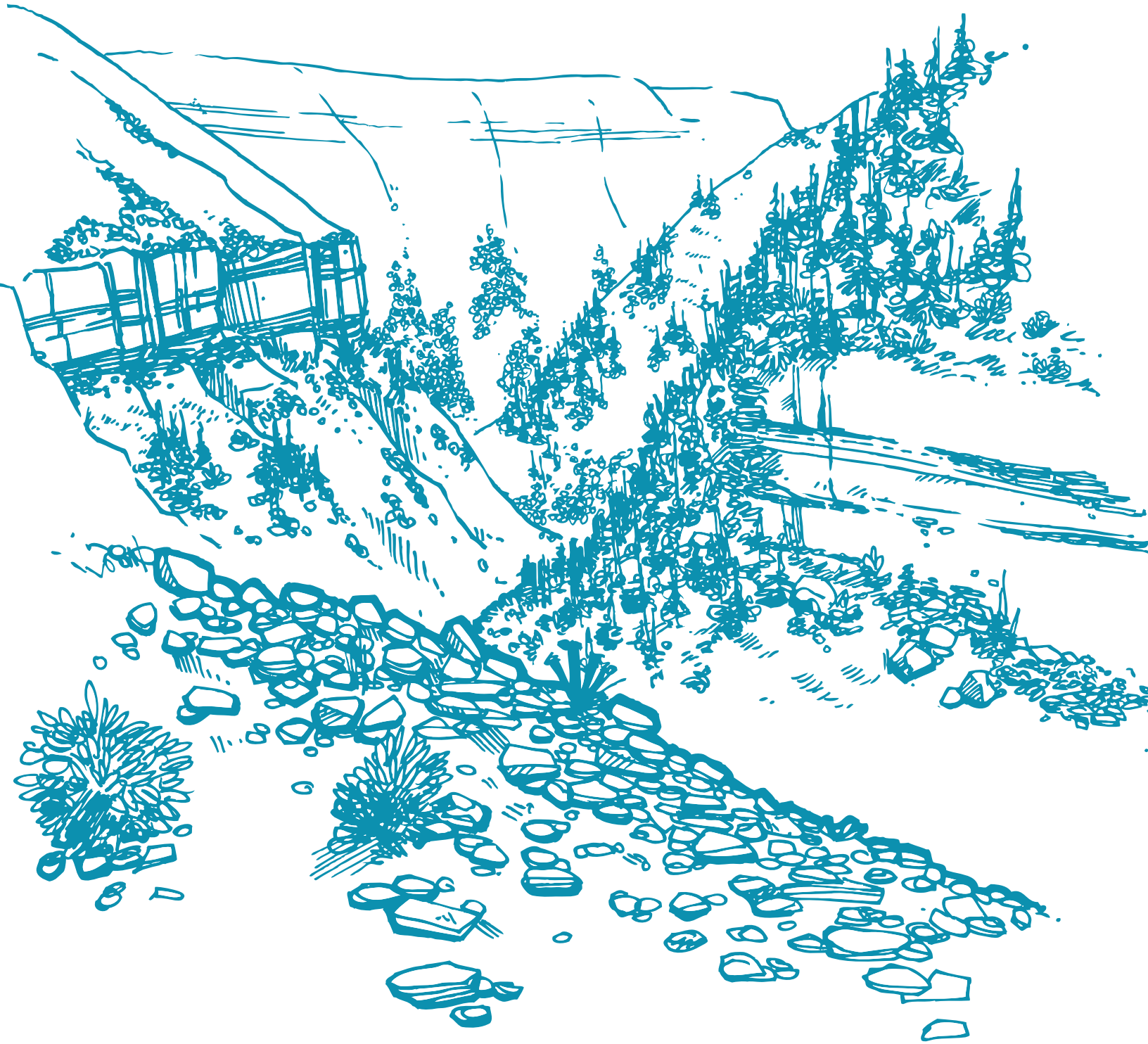
APPENDIX A. Materials distributed at 2011 External Advisory Board Meeting (see attached).

APPENDIX B. Flamelets reaction/mixing model for application in LES (see attached).

ADVISORY BOARD MEETING

2011

THE INSTITUTE FOR CLEAN AND SECURE ENERGY
THE UNIVERSITY OF UTAH



ADVISORY BOARD MEETING 2011

THE INSTITUTE FOR CLEAN AND SECURE ENERGY
THE UNIVERSITY OF UTAH

November 1, 2011
Warnock Engineering Building, Eccles Board Room

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

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

2:30 - 2:50 Break

2:50 - 5:00 Research Project Presentations

- 2:50 Professor Adel F. Sarofim - Oxy-Coal Alstom Boiler Simulation Project
- 3:10 Professor Milind D. Deo - American Shale Oil Project
- 3:30 Professor Lincoln Davies - Carbon Capture & Sequestration: A Regulatory Gap Assessment
- 3:50 Professor Sean T. Smith - Mineralization: The Postcombustion Capture Program
- 4:10 Professor Jeremy N. Thornock - The Oxy-Fuel Combustion CO_2 Capture Project
- 4:30 Professor Eric G. Eddings - Fast Pyrolysis for Hydrocarbon Fuel Production

6:30 - 9:00 Advisory Board Dinner

November 2, 2011
INSCC, Conference Room 345
Closed Session

8:30 - 9:00 Breakfast

9:00 - 10:00 Climate Change Regulation: 2011 Year in Review, Professor Arnold W. Reitze, Jr.

10:00 - 10:20 Break

10:20 - 12:30 Advisory Board Executive Session, Adjourn

Institute for
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THE UNIVERSITY OF UTAH

K. Ian Andrews

Manager of Resource Development Group, PacifiCorp Energy

Mr. Andrews is the manager of the resource development group for PacifiCorp Energy. His current responsibilities include managing the development of the company's self-build options for new wind and gas-based electric power generation resources. He participates in a number of regulatory groups advising on proposed rules regarding carbon capture and sequestration. He has been involved in a variety of functions in the generation sector including project management, air pollution control compliance, plant performance, plant design, contract negotiations, resource planning, due diligence for generation resource acquisition, renewables, IGCC, and new technology assessment. Mr. Andrews has over 30 years experience at PacifiCorp Energy and its predecessors. He holds a degree in chemical engineering from the University of Utah and a business degree from Brigham Young University.

Spencer P. Eccles

Executive Director for the Governor's Office of Economic Development

Spencer P. Eccles became the Executive Director of the Utah Governor's Office of Economic Development in September 2009. Mr. Eccles was formerly affiliated with the Salt Lake City office of Wells Capital Management (Wells Fargo Bank), and has been involved with web-based software and materials technology companies in the U.S. and abroad, chairing the board of the Utah-based company COMPLETExRM and serving as a board member for Swarmbuilder, Inc. and d3o, a materials technology development firm headquartered in the United Kingdom. Mr. Eccles involvement with Utah's non-profit community includes chairmanship of the Salt Lake Chamber's International Committee, serving as president of the First Security Foundation, and advising with The George S. and Dolores Doré Eccles Foundation, Mr. Eccles is also a member of the advisory boards of the Tanner Humanities Center's World Leaders Lecture Forum and the David Eccles School of Business at the University of Utah. Mr. Eccles holds a B.A. in History from the University of Utah and an M.B.A. from Brigham Young University's Marriott School of Management.

James A. Holtkamp

Partner & Manager of the Global Climate Change Practice Group, Holland & Hart

Mr. Holtkamp is the Climate Change Practice Team Leader and the past Manager of the Environmental Compliance Group at Holland & Hart and resident in the Firm's Salt Lake City office. He has actively represented industry and government clients in various environmental, natural resources and energy project development issues throughout the United States and overseas. In particular, Mr. Holtkamp is extensively involved in climate change issues, including avoided deforestation sequestration in Central America, carbon credit trading in the United States, Canada, Latin America and Europe, corporate climate change policies in the energy sector, and development of governmental climate change programs. He has spoken and published widely on climate change in the United States, Canada and Europe. His energy work includes serving as air quality counsel for major electric generation project developers, representation of an independent transmission developer, and work with geothermal operations. He has been general counsel to an electrical utility system and has represented various clients in utility regulatory proceedings. He also has extensive experience in representation of operators of uranium mines, uranium mills, and radioactive waste facilities. Mr. Holtkamp is an adjunct professor of law at the University of Utah, where he teaches the Law of Air Pollution Control and the Law of Climate Change. Mr. Holtkamp holds a B.A. from Brigham Young University and a J.D. from George Washington University.

Hisashi "Sho" Kobayashi

Corporate Fellow, Praxair, Inc.

Dr. Hisashi ("Sho") Kobayashi is Corporate Fellow at Praxair, Inc. (Formerly Union Carbide Corporation). Most of his 33 year career has been dedicated to developing oxygen combustion applications focusing on reducing pollutant emissions and increasing fuel efficiency in industrial furnaces. Applications developed and commercialized include a hazardous waste incineration process, oxy-fuel fired glass melting, aluminum melting and steel reheating furnaces, and oxygen-enhanced NOx reduction process for coal fired boilers. His efforts have resulted in over 60 US patents and over 60 technical papers. Dr. Kobayashi holds a bachelor's degree in Aeronautical Engineering from the University of Tokyo and a M.S. and a Ph.D. in Mechanical Engineering from Massachusetts Institute of Technology.

Robert Lestz

Chief Technology Officer, GasFrac Energy Services

Robert Lestz is a degreed petroleum engineer with 27 years of experience in the oil and gas industry and currently serves as the Chief Technology Officer for GasFrac Energy Services. As the Chief Technology Officer, his organization is responsible for the development of company's R&D, engineering, intellectual property and supporting technical sales. He spent 22 ½ years at Chevron working in the areas of well stimulation, artificial lift, coiled tubing, completions, and remedial well work operations. Robert last led a multidiscipline R&D organization at Chevron's technology company specifically focused on Unconventional Resources. Part of this effort involved building and managing external partnerships at Universities and National Laboratories. He holds 5 patent (including those associated with the GasFrac technology) and has additional patent applications pending. He previously served on the board of directors of the Petroleum Technology Transfer Council and on the United States Department of Energy Oil Shale Ad Hoc Group and is currently on the advisory board of the University of Utah Institute for Clean and Secure Energy. He has also published numerous articles in trade journals and peer reviewed technical journals.

John L. Marion

Director of Global Technology, Alstom Power

Mr. John L. Marion is the Director of Global Technology for Alstom Power's Thermal Products Boiler Business, responsible for R&D worldwide. Mr. Marion was formerly VP of Global Engineering for Alstom Power's Utility Boiler Businesses and has held prior management positions in Strategic Planning, Contract Research Administration, Business Development, and Combustion Research. Prior to taking on management roles, Mr. Marion's research experience was related to emissions control, combustion testing, numerical modeling, and combustion systems product development. Mr. Marion holds B.S. and M.S. degrees in Mechanical Engineering from the University of Massachusetts, as well as an M.B.A. from Rensselaer Polytechnic Institute.

Laura Nelson
Vice President, Energy and Environment, Red Leaf Resources

Dr. Laura Nelson joined Red Leaf Resources, Inc. as its Vice President of Energy and Environmental Development in October 2007. Prior to joining Red Leaf, Dr. Nelson was Energy Advisor to Utah's Governor, Jon Huntsman, Jr., in which capacity she advised the Governor on all aspects of energy policy and emerging alternative technology, including leadership in crosscutting environmental and climate issues. Dr. Nelson participated as a state representative in the review of RD&D proposals for Oil Shale commercial demonstration leases in Utah and as a cooperating agent in the review and evaluation of the Oil Shale and Tar Sands Programmatic Environmental Impact Study. She was responsible for identifying and supporting regulatory projects to promote better land use while realizing increased energy production and improved environmental quality. Prior to serving as Governor Huntsman's Energy Advisor, Dr. Nelson worked as a Policy Strategist for Idaho Public Utilities Commission where she advised the Commission on federal, regional and state energy policy. She performed detailed evaluations on long-term market trends and conditions to assess resource needs, cost assessments and price scenarios. Dr. Nelson is the Chair of the Utah Mining Association Committee on Oil Shale/Sands, a member of the U.S. Department of Energy's Oil Shale Industry Committee, and the former Co-Chair of the U.S. Strategic Unconventional Fuels Task Force. Dr. Nelson holds a B.S. and a Ph.D. in Economics from the University of Utah.

Dianne R. Nielson
Former Energy Advisor, State of Utah

Dr. Dianne Nielson served as the Governor's Energy Advisor for the State of Utah from 2007 to 2011. Dr. Nielson served the citizens of Utah for 27 years, including her prior appointment as the Executive Director of the Utah Department of Environmental Quality and a member of DEQ's five policy Boards. During her career in natural resources, Dr. Nielson directed the Utah Division of Oil, Gas, and Mining; served as a member of the Utah Board of Oil, Gas, and Mining; and worked as Senior Economic Geologist for the Utah Geological Survey. Prior to her work in state government, she conducted energy and mineral exploration with private industry. Dr. Nielson has chaired or worked on numerous state and federal commissions and advisory committees dealing with environmental quality and resource development. Dr. Nielson holds a B.A. from Beloit College, and an M.A. and Ph.D. in geology from Dartmouth College. She is a Licensed Professional Geologist, a Fellow of the Geological Society of America, and a member of the American Association of Petroleum Geologists.

David W. Pershing
Senior Vice President for Academic Affairs, University of Utah

Dr. Pershing is currently a Distinguished Professor and Senior Vice President for Academic Affairs at the University of Utah. Dr. Pershing joined the University of Utah as an Assistant Professor in Chemical Engineering in 1977. He was named a Presidential Young Investigator by the National Science Foundation in 1984 and became Dean of the College of Engineering in 1987. He has had a brilliant career in academia, government, industry and consulting. He has more than 80 peer-reviewed publications, more than 20 research grants, and five patents to his credit. Dr. Pershing has won both the Distinguished Teaching and Distinguished Research Awards and is the 1997 recipient of the Rosenblatt Prize for Excellence. He is the director of the University's Center for Simulation of Accidental Fires and Explosions, fueled by a $20 million grant from the U.S. Department of Energy of Utah. Dr. Pershing holds a B.S. in Chemical Engineering from Purdue University in 1970 and a Ph.D. in Chemical Engineering from the University of Arizona.

Mark Raymond
Uintah County Commissioner

Mark Raymond currently serves as a Uintah County Commissioner. Most recently he served as the Associate Director for USTAR (Utah Science, Technology and Research) for the Eastern Region of the state. Mark is retired from Deseret Generation and Transmission where he was employed as a Lab Technician, Electrical and Controls Technician, and Human Resource Manager. He also served for several years as the Instructor for the Electrical Apprenticeship program taught through the Uintah Basin Applied Technology College. He has also worked for Utah Power and Light, Williams Electric, Halliburton, and Atlas Minerals. Mark has been very active in serving his community in various capacities including: Uintah Impact Mitigation SSD Board member and Vice Chair, Uintah County Planning and Zoning Board member, Department of Workforce Services, past State Council member, and member of the Eastern Region Council, Uintah Basin Applied Technology College, Business Department, Advisory Board member, Vernal Area Chamber of Commerce, Oil and Gas Committee, Education Committee, and Uintah County Sheriff's Advisory Board member. Commissioner Raymond graduated from the University of Utah with two Bachelors of Science Degrees in Psychology and Sociology respectively.

Adel F. Sarofim
Presidential Professor, University of Utah

Dr. Adel F. Sarofim is Presidential Professor in the College of Engineering, University of Utah, co-director of the Utah Clean Coal, and Senior Technical Advisor to Reaction Engineering International in Salt Lake City. He was affiliated with MIT from 1958-1996 as an Instructor in Chemical Engineering in 1958 and 1960; Assistant Professor in Chemical Engineering from 1961-1967; Associate Professor from 1967 to 1972; and Full Professor in Chemical Engineering since 1972. He held the position of Lammot du Pont Professor of Chemical Engineering at MIT from 1989-1996, Emeritus from October 1, 1996. Dr. Sarofim has been a Visiting Professor at Sheffield University, England, the University of Naples, Italy; and at the California Institute of Technology.

Madhava Syamlal
Focus Area Leader of Computational and Basic Sciences, National Energy Technology Laboratory

Dr. Syamlal is currently the Focus Area Leader of Computational and Basic Sciences at NETL. As Focus Leader, Dr. Syamlal is responsible for the development and application of models, atomistic/molecular to device to process scales, and the development of advanced energy systems. Dr. Syamlal has research expertise in multi-phase flow theory and software development, applications of models for dense reacting flow systems, and multi-scale modeling for accelerating technology development. Dr. Syamlal led the development of the internationally recognized open source software for computational multiphase flow MFIX (https://mfix.netl.doe.gov/), which has helped the development of novel physical models and algorithms. Dr. Syamlal also developed a detailed coal gasification/combustion model based on MFIX. The module, called Carbonaceous Chemistry for Continuum Modeling (C3M), is now routinely used at NETL for understanding and designing advanced gasifiers. Dr. Syamlal's research also led to the development of the first commercial software for linking computational fluid dynamics (FLUENT) models with process simulation models (Aspen Plus). The coupling software allows process simulation to include high fidelity device-scale models based on computational fluid dynamics. The higher fidelity process simulation will help engineers to better understand the impact of device-scale behavior on the overall process, and, thereby, speed up technology development. Dr. Syamlal holds a B.Tech, M.S. and PhD. in Chemical Engineering from the Illinois Institute of Technology.

1. ICSE is currently pursuing several collaborative research projects with industry partners, many of which were presented on the first day of this year's Board meeting. Which projects and models of ICSE-industry collaboration appear most promising from the perspective of maximizing the potential for long-term research and funding? Are there alternate approaches to industry research collaborations that ICSE should be considering?

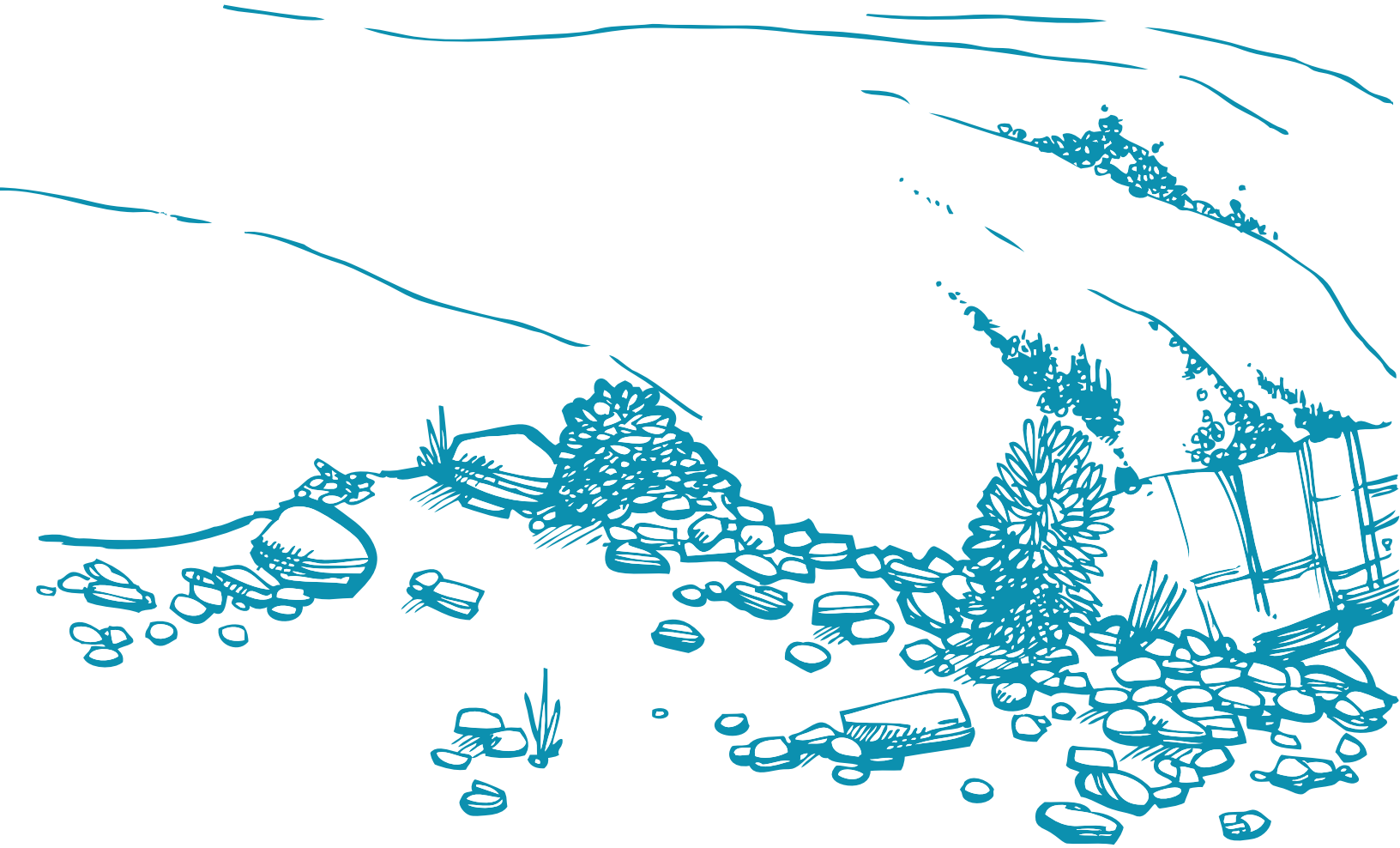
2. What role can the Board play in helping ICSE to develop more collaborative research opportunities with industry?

3. Are there specific areas of research where ICSE should focus its future research efforts with industry?

4. Due to the requirements of the last several years of Congressionally-directed funding ICSE has pursued greater internal inter-disciplinarity, adding legal and economic policy research and public policy forums to its scope of research and activities. In the absence of Congressionally-directed funding, should ICSE continue to pursue this inter-disciplinarity?

5. ICSE has used Congressionaly-directed funding to develop and implement broad research hierarchies composed of several smaller complementary projects all feeding into the larger research agenda. Should ICSE continue to pursue this Institute-wide model of research and funding, or return to an internal model of loosely affiliated individual research and funding opportunities?

6. What concrete steps should ICSE take to generate more research funding opportunities in the impending absence of Congressionally-directed funding?



LES coupled resolved and unresolved combustion model

Consider the generic chemical reaction

$$A^* \rightarrow I + O_2 \rightarrow P$$

Where A* is some element that is *ed, I is the intermediates, O_2 represents the oxidizer, and P is the products.

I. DARS GUI
   a. Use the Flamelet library to create four files needed to begin a simulation
      i. This case only uses 1 Radiation Factor (RF)
      ii. Mixture fraction with 101 points
      iii. Fuel and oxidizer streams are defined
         1. Fuel stream has CSTAR with a value of 0.0 mass fraction
      iv. Four files that are generated
         1. FlameUserSettings.txt
            a. Contains the RF used for a simulation
         2. GasCompoisiton.txt
            a. Contains the Fuel and Oxidizer stream information
         3. InputRedKinMec.txt
         4. InputRedKinTherm.txt

II. Running DARS from script files
   a. Loop over ETA.txt (0.0 to 1.0)
      i. $\eta = \frac{m_{A^*}}{m_{A^*}+m_I+m_{O_2}}$ (1)
      ii. $\eta = 0 \rightarrow all\ CH4$
      iii. $\eta = 1 \rightarrow all\ CSTAR$
   b. Loop over RF.txt (-12.0 to 12.0)
      i. The “good range” needs to be determined
   c. Change the value of CH4STAR and CH4 in the GasComposition.txt file
   d. Change the value of RF in the FlameUserSettings.txt file
   e. Run chamble.exe (DARS solver) for the given settings
   f. Result
      i. ETA folders from (0.0 to 1.0)
         1. Each containing RF (-12.0 to 12.0) folders
         2. Each RF folder contains a range of χ_{st} , starting at a chosen χ_{st} to blowout.
   g. Gather only SV*, and YP* files to be used as the data for the table.
      i. SV* files, contain the information of state space variables (T, density, enthalpy, molecular weight, etc.) as a function of mixture fraction
      ii. Yp* files, contain the mass fraction information of the species of interest in the kinetic file, as a function of mixture fraction

III. Matlab

a. Use the Dan Hinckley model to open and store all the data in a multidimensional array
b. Calculate sensible heat (h_s) from the adiabatic case (RF = 0.0) from each value of η
c. Calculate heat loss (γ):
    i. $\gamma = \frac{H_a - H}{h_s}$ (2)
d. Calculate chi, if the values are not being printed out from DARS.
    i. (Fox, 5.271, 205)
    ii. $\chi = \chi^* \exp\left(-2\left(erf^{-1}(2z-1)\right)^2\right)$ (3)
    iii. Joseph from CDApatco update: Dec 15 should be the distribution day for the new DARS update, which is to include χ as a function of z
        1. Currently using the BETA version of DARS v 2.08.005
e. Include h_s and h_a in the table
f. Include χ_{min} and χ_{max} in the table
g. Use matlab function " TriScatteredInterp" do perform multi-variable interpolation
    i. Can only have a max of 3D
        1. Interpolate over (χ,z, γ)
    ii. Interpolate/Extrapolate in heatloss space, in order to have a "good range" for the TirScatteredInterp matlab function
    iii.
h. Calculate the equations for the "one-time marginal PDF's of mixture fraction and scalar dissipation rate"
    i. mixture fraction PDF
        1. β-PDF or clipped Gaussian
    ii. scalar dissipation rate PDF, note: (μ and σ) are unknown
        1. $f_{\chi^*} = \frac{1}{\sigma(2\pi)^{\frac{1}{2}}} \frac{1}{\chi^*} exp\left[-\frac{1}{2\sigma^2}(ln(\chi^*) - \mu^2)\right]$ (4)
            a. Where μ is related to the mean value of χ^*
            b. And σ is related to the standard deviation (variance)
                i. From experimental work σ = [2, 4], Fox pg. 206
            c. Get a range on the values of $\langle\chi\rangle$
            d. Solve for the range on $\langle\chi^*\rangle$ by:
            e. $\langle\chi\rangle = \langle\chi^*\rangle * \langle exp(-2[erf^{-1}(2z-1)]^2)\rangle$ (5)
                i. Try to use matlab functions to integrate 2nd term on RHS.
            f. Determine the value of μ for each $\langle\chi\rangle$
                i. $\langle\chi^*\rangle = exp(\mu + 0.5\sigma^2)$ (6)
            g. Use the Joint mixture Fraction , dissipation rate PDF result to get the correct
            <Φ > (variable of interest)
            h. $f_{z,\chi} = f_z f_{\chi^*}$ (7)
            i. $\langle\phi\rangle = \int_0^1 \int_0^\infty \phi\, f_{z,\chi} d(\chi) d(z)$ (8)

i. Use a matlab quartier integrator to perform integration (equation (8))

IV. ARCHES/LES

a. $\langle \chi \rangle = C_{\tau,SKE} \frac{Z_v k^{\frac{1}{2}}}{\Delta}$ (9)

i. Z_v is the mixture fraction variance

ii. $C_{\tau,SKE} = 2$

iii. z_v = g

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