Attachment 2 - Statement of Program Objectives
Clean and Secure Energy from Domestic Oil Shale and Oil Sands Resources

This Statement of Project Objectives (SOPO) reflects the performance period from October 1, 2010 through September 30, 2013. It includes tasks/subtasks funded in fiscal year 2009 (Phase 1) and tasks/subtasks funded in fiscal year 2010 (Phase II). Tasks/subtasks initiated during Phase I that are anticipated to continue in Phase II shall satisfactorily meet Phase I deliverables and milestones as described in the SOPO and Project Management Plan (PMP), respectively, prior to continuation to Phase II.

A. OBJECTIVES

The University of Utah (the Recipient), via their Institute for Clean and Secure Energy (the Institute), shall pursue research to improve industry’s ability to utilize the vast energy stored in domestic oil shale and oil sands resources in a manner that shall minimize environmental impact from production.

The project has three overarching project objectives:

1. **Basin scale simulation of environmental and economic impacts of oil shale & oil sands development**
   The objective of this project area is to produce the research and simulation tools needed to assess liquid fuel production, upgrading, and refining from oil shale and oil sands, and specifically to produce basin/regional scale simulation tools with predictive capability for evaluating the potential for unconventional resource development given a range of environmental and economic constraints.

2. **Secure liquid fuel production by in-situ thermal processing of oil shale & oil sands**
   The objective of this project area is to apply science, engineering, technology and economics research tools developed within the Institute to a wide variety of in-situ processes and to explore the environmental, legal and policy framework for implementation of such technologies on public and private lands.

3. **Environmental, Legal, and Policy Issues**
   There are two main objectives in this project area: (1) to explore and identify gaps in the environmental, legal and policy framework for implementation of in-situ thermal processing technologies for oil shale and oil sands on public and private lands and (2) to perform an economic and policy evaluation of domestic oil shale and oil sands development.

B. SCOPE OF PROJECT

The technical research program, organized around the theme of validation and uncertainty quantification through tightly coupled simulation and experimental designs, is integrated with the legal, environment, economics and policy research program to
achieve the dual goals of clean and secure energy from domestic oil sands and oil shale resources.

The research targets include:

- Basin scale oil shale and oil sands development – Advanced technologies have the potential to provide improved economics while reducing the environmental impact and carbon footprint associated with the development of unconventional resources. This validation research brings experimental data and process model simulations, life-cycle greenhouse gas (GHG) analysis, and data from various Utah agencies into the CLEAR$_{uff}$ framework to produce a tool with quantified predictability that can then be applied to the assessment of basin-/regional-scale impacts of oil shale and oil sands development.

- In-situ thermal processing – In-situ technologies are currently being explored because of their potential for reducing the environmental footprint of oil shale/sands development. The objective of this research is to create models and simulation tools that shall apply to all in-situ thermal processes. Practitioners could then use the tools to optimize their process for energy efficiency, to evaluate various heating strategies, etc. This objective shall be achieved by utilizing oil shale core samples recently obtained by the Institute from the Skyline 16 drill site on private land in the Uinta Basin. Fresh core samples shall provide “standard samples” to the experimental research being conducted on multiple scales. Using this experimental data (including geomechanical, geochemical, structural, and pyrolysis data), simulation tools necessary to capture the relevant physical processes shall be refined. Data from industrial sources and from Institute laboratories shall be used for validation/uncertainty quantification (V/UQ) conducted at multiple scales.

- Environmental, legal, economic & policy framework – This research shall address legal, policy and economic gaps that pertain to in-situ liquid fuel production from oil shale/sands. It shall address the natural hydrologic connection between surface and groundwater by analyzing conjunctive management of these resources, gaps in regulation, and what implications the legal framework for conjunctive management has for oil shale and sands development. It shall address cross-jurisdictional resource management given the myriad of non-federal landowners and managers who control access to significant quantities of oil shale and sands and shall seek to identify resource areas with the highest development potential in light of existing resource assessment constraints. This research shall also review existing legal issues and constraints relevant to the use of simulation for environmental risk assessment/impacts analysis to provide policymakers with analysis of the perceived and practical sufficiency of simulation in such a context.

C. TASKS TO BE PERFORMED

Task 1.0 – Project Management and Planning

The Recipient shall execute the project in accordance with the approved Project Management Plan (PMP) covering the entire project period. The Recipient shall manage
and control project activities in accordance with their established processes and procedures to ensure subtasks and tasks are completed within schedule and budget constraints defined by the Project Management Plan. This management includes tracking and reporting progress and project risks to DOE and other stakeholders.

The Recipient shall work together with the DOE Project Officer to develop and submit a PMP. The PMP is a stand alone document that shall include a work breakdown structure and supporting narrative for each task and subtask, as identified in the Statement of Project Objectives. This narrative shall concisely describe the research and analytical approaches or methods the Recipient shall use to achieve the objectives of each task/subtask and the cost and schedule necessary to complete each task/subtask. The Recipient shall also provide in the PMP a milestone log that describes milestones and their relationship to specific tasks and subtasks. Each milestone shall include a planned completion date that shall be tracked as part of the quarterly Progress Report.

The PMP shall be submitted within 30 days of the award. The DOE Project Officer shall have 20 calendar days from receipt of the PMP to review and provide comments to the Recipient. Within 15 calendar days after receipt of the DOE’s comments, the Recipient shall submit a final PMP to the DOE Project Officer for review and approval.

The Recipient shall review, update, and amend the PMP (as necessary as requested by the DOE Project Officer) at key points in the project, notably at each major Task/Subtask Decision Point and upon schedule variances of more than 3 months and cost variances of more than 15%, which require modifications to the agreement and which constitute a re-baselining of the project.

**Task 2.0 – Technology Transfer and Outreach**

This task shall focus on industry, academic and public outreach and education efforts, as well as continued efforts to integrate research and to gather and implement recommendations from the Recipient’s External Advisory Board (EAB). The Recipient shall coordinate and arrange meetings of the EAB in order to garner continued feedback on means by which the Recipient can enhance its research and outreach efforts. The EAB shall meet formally on an annual basis. The EAB shall provide input in the selection of Institute-sponsored tasks/projects and, together with DOE, provide annual review of ongoing tasks/projects. The purpose of the EAB is to direct the overall mission of the Institute, and the composition of the EAB reflects the diversity of work occurring within the Institute. If additional direction is needed for certain targeted groups, the Recipient shall consult informally with ad hoc technical advisors.

The Recipient shall engage in an enhanced dialogue with industry through programs such as fellowships, plant trips, and papers published in trade journals. With a fellowship program, industry shall have a mechanism to fund student work within the Institute. Plant trips provide an opportunity for students and faculty to better understand energy generation and fuel production at the largest scales. Publication of ongoing research results in scientific and trade journals will enhance the Institute’s visibility, connect research results to industry and other interested stakeholders, and improve public awareness with respect to the economic, technical, legal, and political complexity of developing the nation’s unconventional fuel resources.
The Recipient shall also pursue outreach opportunities at both a technical and a public level to foster discussion of energy policy issues and the role of unconventional fossil fuels in the nation’s energy portfolio. The Recipient shall organize and hold the Unconventional Fuels Conference and the ICSE Energy Forum in order to educate the public, engage various stakeholders, and effectuate better understanding of Recipient’s scientific and policy research activities. The Recipient shall also organize and hold workshops and topical seminars to better facilitate interdisciplinary integration of research and analysis and to encourage the flow of information among government, industrial, academic, and public constituencies. Lastly, the Recipient shall work with librarians at the University of Utah’s Marriott Library to transition the repository from the DSpace platform currently housed on Institute servers to a stand-alone digital collection housed in the Marriott Library. This will ensure continued access to the materials currently housed in the repository related to unconventional fuel resources in North America with a regional emphasis on the western U.S.

Task 3.0 Basin scale simulation of environmental and economic impacts of oil shale & oil sands development

The ultimate goal of the task is to develop a predictive tool for assessing the basin- or regional-scale environmental and economic impacts of unconventional fuel development. To achieve this goal, the Recipient shall assess advanced technologies such as oxy-gas process heater technology to reduce the carbon footprint of unconventional fuels development. The Recipient shall develop an integrated assessment model such as CLEAR for evaluating life-cycle greenhouse gas emissions, water requirements, and economic impacts for a range of processes at a range of scales. V/UQ research shall establish the predictive capability of the simulation tools that are developed.

The Computational Earth Sciences Group at Los Alamos National Laboratory (LANL) has recently developed the dynamic, integrated assessment model CLEAR to evaluate the potential for unconventional fuel development given environmental and economic constraints such as water availability, land use regulations, and size of the local labor pool. Dr. Donatella Pasqualini, the primary developer of CLEAR, shall provide guidance to Subtasks 3.1 and 3.2 in developing and implementing new modules into CLEAR. In addition, Dr. Pasqualini shall work closely with researchers in Subtask 3.4 so that they understand the overall features, coding practices, verification methodologies, inputs, boundary conditions, information flow, and solution methodologies employed in CLEAR. Finally, she shall help identify the parameters to test in the V/UQ study and shall serve as a CLEAR resource throughout the project.

Subtask 3.1 – Life-cycle greenhouse gas analysis of conventional oil and gas development in the Uinta Basin

The Recipient shall collect available experimental, literature, and simulation data on GHG emissions from oxy-fuel flameless process heaters. This data shall complement the information collected previously by the Recipient on the GHG emissions from several electricity generation and liquid-fuel production technologies. During Phase I of this subtask the Recipient shall also develop or modify an existing model for evaluating life-
cycle GHG emissions at a range of scales. A collection of this life-cycle GHG emissions data shall be added to the Institute repository.

Task Deliverable (Phase I): The Recipient shall use the model for life-cycle GHG emissions to compare an upgrader or refinery with oxy-fuel flameless process heaters with those from an operation with conventional process heaters. Model results will be provided to DOE/NETL in a Topical Report. The report shall include a summary of model parameters and referenced data sources.

Subtask Decision Point - Continuation to Phase II activities shall be dependent on satisfactory completion of task work and deliverables associated with Phase I efforts as described above, and approved by the NETL Project Officer.

The long-term goal of this work shall be to develop a predictive tool that provides probability distributions of life-cycle GHG emissions from various upstream and downstream energy-production technologies. During Phase II of this subtask, the Recipient shall incorporate life-cycle GHG emissions modules for conventional oil and gas development in Utah’s Uinta Basin into CLEARuff. The Uinta Basin, a region with immense oil shale and oil sands resources, is also the location of a recent conventional oil and gas boom. This task aims to apply V/UQ methodologies to the development of this life-cycle GHG predictive tool for unconventional fuel processes using available conventional fuel data from the Uinta Basin.

The Recipient shall collect available experimental and literature data on GHG emissions associated with the drilling and production of conventional oil and gas. Basin-specific information shall be obtained from available sources, including the Utah Division of Oil, Gas, and Mining and the Utah Division of Air Quality (DAQ). The Recipient shall develop the overall system dynamics, module couplings, and model parameters that shall be explored and integrated into the CLEARuff model.

Task Deliverable (Phase II): The Recipient shall provide modules in CLEARuff for life-cycle CO₂ emissions from conventional oil and gas development in the Uinta Basin, and the results will be provided to DOE/NETL in a Topical Report. The report shall include a summary of results and referenced data sources.

Subtask 3.2 – Flameless oxy-gas process heaters for efficient CO₂ capture

The Recipient shall create a Large Eddy Simulation (LES) tool for demonstrating practical oxy-gas flameless combustion in process heaters and then use that technology to produce predictive capability with quantified uncertainty bounds for large-scale (pilot or commercial), flameless, oxy-gas process heaters. Particular attention shall be focused on flameless operation for different process heater design options burning a wide range of gaseous fuels including natural gas, refinery gas, and the by-product gas stream produced from in-situ oil shale/sands production. Oxy-gas flameless combustion experimental data sets at the pilot- or commercial-scale shall be identified. Two likely candidates are data sets from CANMET and from the International Flame Research Foundation. The LES tool developed for this project shall be applied to one of those data sets to demonstrate the process of validation and uncertainty quantification in such systems.
Task Deliverable (Phase I): The Recipient shall provide a completed Validation/Uncertainty Quantification Analysis of an oxy-gas combustion system in a Topical Report to DOE/NELT that summarizes results and lessons learned.

Subtask 3.3 – Development of conventional oil and gas production modules for CLEAR

Subtask Decision Point - Commencement of this subtask shall be dependent on satisfactory completion of work and deliverables associated with Phase I of subtask 6.1 as described below, and approved by the NETL Project Officer.

The Recipient shall develop process models for conventional oil and gas drilling, production, transportation, management of produced water, and infrastructure development in the Uinta Basin. The process models calculate flows of material, heat, energy, water and pollutants as well as fixed and operating costs for the process. A specific focus of this task shall be the development a produced water process model that includes options for treatment, use, and/or disposal of produced water. These models shall be coupled with the life-cycle GHG emissions work from Subtask 3.1 and implemented as conventional oil and gas and as produced water modules in the CLEAR framework. Available data from the Utah Division of Oil, Gas, and Mining, from Uintah County, and from other regulatory agencies shall be used to perform a V/UQ analysis on these process models to quantify the uncertainty in model parameters and outputs.

Task Deliverable (Phase II): The Recipient shall provide modules in CLEAR for conventional oil and gas development and for produced water management in the Uinta Basin. Additionally, the Recipient shall submit a Topical Report to DOE/NELT that include a summary of the process models developed, V/UQ results for the process models, and referenced data sources.

Subtask 3.4 – V/UQ analysis of basin scale CLEAR assessment tool

The Recipient shall develop a first generation methodology for doing V/UQ on system models like CLEAR that is based on a methodology developed in the Institute for multi-scale, multi-physics processes. Issues that shall be considered include (1) how to systematically determine which of the hundreds of model parameters have the largest effect on outputs of interest such as energy and water demand, (2) what is the distribution of uncertainty ascribed to the various parameters and how can that choice be justified, and (3) how to perform V/UQ on a dynamical system (look at snapshot at a single moment in time, track a pattern over time, etc.). The Recipient shall demonstrate an application of methodology for conventional oil & gas development during the recent (2000-2008) Uinta Basin oil boom, specifically focusing on changes in water and energy demand, population, and tax revenues.

Task Deliverable (Phase II): The Recipient shall submit a Topical Report to DOE/NELT describing the V/UQ methodology applied to CLEAR and the lessons learned from its application to conventional oil and gas production in the Uinta Basin.

Task 4.0 - Liquid fuel production by in-situ thermal processing of oil shale/sands
The ultimate goal of this task is to create tools to implement environmentally responsible technologies for the development of unconventional resources. The Recipient shall perform research to generate data and to create numerical models and simulation tools that shall apply to all in-situ thermal processes for oil shale/sands liquid fuel production and shall gather experimental laboratory data on multiple scales. The process of V/UQ quantification shall then be applied to specific laboratory- and pilot-scale systems.

In a previous phase of the project, the Recipient obtained 1000 feet of oil shale core from the Skyline 16 drill site. Selected portions of this Skyline 16 core shall be designated as the “standard” material and shall be used in Subtasks 4.3-4.9. Handling protocols shall be established for the standard samples. Additional elemental, mineralogic, and geologic analyses of the core shall be conducted in Subtask 4.8. A portion of the standard core material shall be demineralized and the bitumen and kerogen material obtained through this process shall be designated as “standard” samples for chemical characterization.

As part of the various subtasks described below, the Recipient shall (1) develop a set of standard measurements for fresh core samples that shall be used to develop a comprehensive set of data for model validation and future reference and (2) develop and manage a data repository to store all the relevant data obtained in studies of this new fresh core.

Subtask 4.1 - Development of CFD-based simulations tool for in situ thermal processing of oil shale/sands

The overall objective of this effort is to produce simulation tools with quantified predictivity that can be used by industry to assist in the assessment of the technological, economic and environmental consequences of the production of new gas and liquid fuels from U.S. oil shale/sands deposits. While the Recipient shall specifically apply the simulation tools to Red Leaf Resources patented EcoShale process, the resulting simulation tools and the V/UQ from this work are intended to be applicable to most thermal treatment processes that employ indirect heating: in-situ, modified in-situ or ex-situ.

To accomplish this task, the Recipient shall examine two possible simulation tools; ARCHES and the commercial code Star-CCM+. This phase of work shall build upon previous work for simulating dense two-phase flows. ARCHES development shall include the exploration of the direct quadrature method of moments approach for simulating the solid phase. Development for the Star-CCM+ code shall cover any needed preprocessing methods to define rubblized bed processes, including the generation of a computational mesh, Current efforts are exploring thermal heating of the oil shale using temperature data from Red Leaf.

Task Deliverable (Phase I): The Recipient shall provide a completed Validation/Uncertainty Quantification Analysis in a Topical Report to DOE/NETL that summarizes results and lessons learned.

Subtask Decision Point - Continuation to Phase II activities will be dependent on satisfactory completion of task work and deliverables associated with Phase I efforts as described above, and approved by the NETL Project Officer.
In Phase II of this research, the Recipient shall expand the modeling to include reaction chemistry and study the product yield as a function of operating conditions.

Task Deliverable (Phase II): The Recipient shall distribute software over the web including: (1) ARCHES and (2) all requisite input files and user-defined subroutines for CCM+. The Recipient shall also submit a Topical Report to DOE/NETL on the lessons learned from the optimization/UQ study of product yield as a function of operating conditions for indirectly heated, rubblized oil shale beds.

Subtask 4.2 - Reservoir simulation of reactive transport processes

The ultimate objective of this subtask is to create a reactive-transport reservoir simulation tool capable of modeling the conversion of kerogen to oil and gas and the transport of multiple phases under realistic geologic and reservoir conditions. This tool can then be used to analyze how reservoir heterogeneity impacts production from the Utah oil shale resource.

In Phase I, the Recipient shall build a more effective reservoir simulation tool by managing processes occurring at vastly different temporal scales (for example, reactions versus advance of the thermal front) and by incorporating processes at very small length scales (pore scale, block scale, etc.) into models operating at inter-well or reservoir scale. Information on kinetics of shale transformation from Subtask 4.3 and on pore-level properties from Subtask 4.5 shall be incorporated into the reservoir models. Hence, detailed geologic and reservoir characterization shall be a component of this task.

Task Deliverable (Phase I): The Recipient shall submit at least one paper on in-situ reservoir models with rigorous reaction models for publication in a scientific or industry trade journal.

Subtask Decision Point - Continuation to Phase II activities will be dependent on satisfactory completion of task work and deliverables associated with Phase I efforts as described above, and approved by the NETL Project Officer.

In Phase II, the Recipient shall refine submodels developed during Phase I research using the physical understanding developed in other tasks and shall validate the model using data from Subtask 4.7. Specifically, the Recipient shall 1) incorporate kinetic and composition models developed in Subtask 4.3 into an appropriate reservoir modeling framework, 2) validate the model at a small scale using data from core experiments from Subtasks 4.3 and 4.7, 3) examine various pore-level change models and their impact on the production process, including analysis of data from Subtask 4.5, and 4) utilizing new geologic analysis and mapping from Subtask 4.8, create reservoir models in promising Utah locations by simulating a variety of in-situ processes to identify the technical advantages and challenges of selected processes.

Task Deliverable (Phase II): The Recipient shall distribute software over the web for a thermal reactive model for oil shale that includes complex reaction kinetics. The Recipient shall also submit a Topical Report to DOE/NETL on the validation results for core-scale oil shale pyrolysis.

Subtask 4.3 – Multiscale thermal processes
The use of simulation to evaluate in situ production processes for unconventional fossil fuels requires development of submodels that accurately describe the relevant physical processes that take place at depth, where pore pressure can range from a few atmospheres to several hundred. This subtask focuses on submodel development at two scales. First, the Recipient shall perform fundamental experimental studies to measure the kinetics of transformation of the organic matter in shale and shall develop models that are consistent with all of the measured data.

During Phase I, the Recipient shall build on previous thermal gravimetric analysis (TGA) and bench scale experiments on cores of different sizes to create mechanistic pathways for the conversion of kerogen to oil. Comprehensive characterization performed on the samples from both TGA and bench-scale experiments (gas chromatography, mass spectrometry, NMR, HPLC, density, viscosity, refractive index, elemental analysis, etc.) shall provide the data necessary to develop and refine the kerogen conversion mechanism. Experiments on different sized core samples shall be performed under a variety of conditions and heating rates. An apparatus to study in-situ reactions at pressure and stress shall be designed and built. Data from larger, pilot-scale experiments shall be compiled and compared with laboratory data. Kinetic models of oil shale pyrolysis developed as part of this task shall be validated using data generated in this task and data from pilot-scale experiments.

Task Deliverable (Phase I): The Recipient shall submit two papers for publication in a scientific or industry trade journal; one on the kinetics of oil shale pyrolysis and the other on compositional aspects of the kerogen to oil (and gas) transformation.

Subtask Decision Point - Continuation to Phase II activities will be dependent on satisfactory completion of task work and deliverables associated with Phase I efforts as described above, and approved by the NETL Project Officer.

The Recipient shall conduct thermogravimetric analyses (TGA) experiments of oil shale initiated in Phase I utilizing the fresh "standard" core. These non-isothermal experiments conducted for a range of heating rates shall provide the time-temperature histories required for model development.

Second, the Recipient shall pyrolyze core samples at various pressures and shall analyze the products in detail for bulk properties and composition to determine how heat and mass transfer considerations come in to play apart from the fundamental reaction kinetics. The Recipient shall pyrolyze ¾-inch or 1-inch cores over a range of temperatures and heating rates. Data on oil yield, gas production and coke formation shall be gathered and compared with TGA data. Oil properties, including densities, viscosities (with temperature), pour point, etc. shall be measured. Compositions of the collected oil and gas samples shall be measured using GC. Selected mass spectrometric experiments shall also be conducted. These data shall be used to develop a model that accounts for heat and mass transfer effects in predicting product yields and compositions and to validate the reactive transport reservoir model in Subtask 4.2. Research under this subtask shall be performed jointly with researchers at Brigham Young University (BYU).
Task Deliverable (Phase II): The Recipient shall distribute software over the web for a CPD/shale model and for an oil generation model that is used in the reservoir simulation model. A Topical Report describing these models and their applications/limitations shall be provided to DOE/NETL.

Subtask 4.4 – Effect of oil shale processing water composition

The Recipient shall continue pyrolysis experiments of Green River oil shale with representative of the amounts of water and shall study the resulting water chemistry. Experiments shall be conducted at temperatures ranging from 300’-450’F, heating rates from 0.5-10’F/min, and pressures from atmospheric to 1000 psia. Analytical techniques to be employed for studying organic species in the water include gas chromatography and gas chromatography-mass spectrometry. A small set of samples shall also be analyzed for inorganic species.

Task Deliverable (Phase I): The Recipient shall provide tables of aqueous-phase organic species concentrations to DOE/NETL. The tables shall also be uploaded to the Institute repository for use by internal and external researchers considering the impacts of oil shale processing on groundwater.

Subtask 4.5 – In situ pore physics

This subtask focuses on the study of pore scale transport processes during pyrolysis of oil sands and oil shale by multiscale, three-dimensional (3-D) X-ray computed tomography analysis coupled with Lattice Boltzmann (LB) simulation. The Recipient shall identify critical fundamental factors of pore geometry and structure that limit recovery of hydrocarbons from oil sands and oil shale.

Phase I research objectives include (1) CT analysis of the pore network structure of selected oil shale/sand samples, including residual reaction products during pyrolysis reactions at different temperatures, and (2) multi-phase LB simulations of fluid transport in these porous structures based on the analysis of capillary phenomena. By modeling the pore network structure at different heating rates, information such as porosity change shall be provided to Institute researchers developing scale-bridging models for multiphase flow. Results obtained from multiphase LB simulations shall provide transport information such as connectivity, conductivity, and permeability to scale-bridging models and to reservoir simulation tools.

Task Deliverable (Phase I): The Recipient shall provide a Topical Report to DOE/NETL describing the results obtained from multiphase LB simulations.

Subtask Decision Point - Continuation to Phase II activities will be dependent on satisfactory completion of task work and deliverables associated with Phase I efforts as described above, and approved by the NETL Project Officer.

In Phase II, the Recipient shall expand work conducted under Phase I by conducting experiments utilizing the new Skyline 16 oil shale samples from Subtask 4.3. The Recipient shall determine directional (anisotropic) permeability for pyrolysis reactions at different temperatures based on the pore network structure determined by X-ray micro
CT (XMT) analysis coupled with LB simulation. The Recipient shall also compute permeabilities of the pyrolyzed core samples under different loading conditions.

Task Deliverable (Phase II): The Recipient shall provide pore network structures and permeability calculations (directional/anisotropic, mineral zones, loading conditions, and temperatures of pyrolysis including heating rate) to Subtasks 4.3 and 4.7. The Recipient shall also submit a Topical Report to DOE/NETL summarizing the results of the study.

Subtask 4.6 - Atomistic modeling of oil shale kerogens and oil sand asphaltenes

During Phase I, the Recipient shall establish representative three-dimensional models of kerogen and asphaltenes. The three-dimensional models shall be used to calculate interaction energies between organic components and the mineral matrix. The Recipient shall correlate analytical spectroscopic data (NMR, IR, X-ray, Mass Spectroscopy, etc.) of the isolated and absorbed three-dimensional models and shall establish sensitivities to the structural features in the models. Through this research, the Recipient shall seek to provide molecular-scale structural and yield information to micro-scale models for pore structure development and kerogen pyrolysis kinetics.

Using information from other team members relating to water composition, pore properties, and oil shale pyrolysis, the Recipient shall provide potential product distribution yields of pyrolysis products by general type, information on aggregation of asphaltenes in oil sands and of bitumen/inorganic material, and analytical data on kerogen and asphaltene structures. Molecular models of kerogen and oil sands bitumen developed in this subtask shall be correlated with organic fragments identified in Subtask 4.3.

Task Deliverable (Phase I): The Recipient shall provide a Topical Report to DOE/NETL describing the results of the three-dimensional modeling including product distribution yields from pyrolysis.

Subtask Decision Point - Continuation to Phase II activities will be dependent on satisfactory completion of task work and deliverables associated with Phase I efforts as described above, and approved by the NETL Project Officer.

In Phase I of the project, the Recipient shall demonstrate molecular modeling techniques for building three-dimensional (3-D) models of kerogens, asphaltenes and their composite models, including mineral matrices. In Phase II, the Recipient shall continue research to establish the validity of 3-D models of kerogen and asphaltenes by performing different molecular mechanics minimizations of two-dimensional models followed by simulated annealing to generate new structures, thus establishing the sensitivity of the final structure to the methods used in its determination. Experimental data obtained as part of Subtask 4.9 (not available during Phase I), including solid and liquid state $^{13}$C NMR spectroscopy, magnetic resonance imaging, TGA data on pyrolysis kinetics, small angle X-ray scattering, and ion cyclotron resonance-mass spectroscopy (ICR-MS) via atom pair distribution function analysis, shall be used to correlate computational results and to validate and verify the various models.
The Recipient shall also continue to model the interaction of kerogen and asphaltene structures with the inorganic matrix using molecular mechanics minimization of the established 3-D structures sandwiched between slabs of illite. Data from Subtask 4.9 shall be used to validate these models. Subsequent to validation, the objective of this modeling is to understand the nature of these interactions so that new approaches can be designed that more readily facilitate the extraction of kerogen from oil shales and of asphaltenes from sand tars without resorting to costly thermal processes.

Finally, the Recipient shall initiate the creation of entirely different models for other shale kerogens such as kukersite. The concept is to create a repository where people working in kerogen-related research activities can easily pull up the structures depending on where the sample was mined. New structures shall be added to this repository once optimal structures have been determined through molecular mechanics.

Task Deliverable (Phase II): The Recipient shall create a repository of 3-D models of Uinta Basin kerogens, asphaltenes, and complete systems (organic and inorganic materials) that is accessible on the web. Additionally, the Recipient shall submit a paper to a journal for publication that describes the development and validation of the 3-D models.

Subtask 4.7 - Geomechanical reservoir state

The Recipient shall perform experiments to replicate in-situ production processes and determine the potential for creation of supplementary permeability and porosity; to evaluate potential methodologies for increasing contact area in the reservoir; and to determine thermophysical properties for complimentary simulations. A unique high pressure-high temperature vessel and an ancillary flow system shall be designed and fabricated to carry out measurements representing oil shale response under realistic in-situ pressure and stress conditions when high temperature in-situ processes are applied. Measurements shall be designed to assess strength, fracturing potential, fracture and matrix porosity creation and yield as well as basic temperature-dependent thermophysical properties required for various simulations.

Acknowledging the anticipated difficulties in performing high temperature, moderate pressure measurements, the Recipient shall develop an experimental matrix to prioritize the measurement program in conjunction with other subtask leaders in this project area. Examples of tests to be performed include (1) thermal loading measurements to duplicate generic in-situ temperature profiles under static but representative in-situ stress conditions and to assess the consequences of the stresses and temperatures on generation of fracture and matrix porosity and permeability, (2) temperature-dependent thermophysical properties required for simulations including thermal conductivity and diffusivity, (3) temperature-dependent thermomechanical properties required for simulations as a function of process history including the coefficient of thermal expansion.

Task Deliverable (Phase II): The Recipient shall provide thermophysical and geomechanical property data to Subtask 4.2 and shall provide validation data for Subtask 4.5. The Recipient shall also submit a Topical Report to DOE/NELT assessing subsidence and compaction implications for assurance purposes with respect to in situ development of oil shale and oil sands.
Subtask 4.8 – Developing a predictive geologic model of the Green River oil shale, Uinta Basin

In order for the Uinta Basin to be more seriously considered as an economic production target, the geologic knowledge gap must be closed. The lateral and vertical heterogeneity of the oil shale intervals in terms of lithology (rock type), mineralogy, and geochemistry is not known, a sequence stratigraphic framework has not been developed, and Uinta Basin history, evolution, and stratigraphy have not been linked to adjacent basins. Lateral and vertical changes in oil shale mineralogy, geochemistry, and geomechanical behavior may result in varying preferred production methods and recovered hydrocarbon products, as well as differences in spent shale composition by region or oil shale zone.

The Recipient shall examine vertical and lateral variability in oil shale properties across a 30-mile N-S transect of the Uinta Basin. This research shall complement previously funded research to build and E-W cross-section through the same area of the basin. Emphasis will be placed on identifying changes in oil shale richness and inorganic mineralogy in order to build a predictive model of behavior across a wide area of the basin that can provide key direction for citing of prospective in situ operations.

The Recipient shall conduct detailed sedimentologic and stratigraphic analysis of three cores, including Skyline 16. The Recipient shall also conduct detailed mineralogic and geochemical analysis of the same cores. Each core shall be sampled stratigraphically and analyzed using X-Ray fluorescence. Additional detailed geochemical analysis shall be performed on the Skyline 16 core, including elemental analyzer-MS, which provides Total Organic Carbon and bulk organic carbon isotope values, A proxy for environmental and climatic change through the succession. X-ray diffraction (XRF) and QEMScan analysis shall be performed on a select number of samples from Skyline 16 to ground truth quantitative XRF data and provide detailed mineralogic data that can be mapped/imaged and analyzed quantitatively/statistically.

Task Deliverable (Phase II): The Recipient shall upload all data and models to a repository, including the detailed core logs, the geochemical analyses, and the cross-sectional diagrams and maps of the geologic model for the basin. The Recipient shall submit a Topical Report to DOE/NETL containing methods and results.

Subtask 4.9 – Experimental Characterization of Oil Shales and Kerogen

The Recipient shall initiate an intensive study of the kerogen structure utilizing the “standard core” that was recently obtained from the Uinta Basin (Skyline 16). A portion of the “standard core” material shall be crushed, homogenized and demineralized by standard techniques to extract bitumen and kerogen. This bitumen and kerogen material shall then be designated as “standard” samples for chemical characterization. The bitumen shall be analyzed by high resolution/high field nuclear magnetic resonance (NMR) techniques, GC-MS, IR, and ion cyclotron resonance (ICR at the National High Field Magnet Laboratory). The structure of the solid kerogen shall be studied by solid state NMR techniques, by small angle x-ray scattering via atom pair distribution function analysis (at Argonne National Laboratory) and by ICR-MS. These data shall be used to correlate computational results and to determine pore structure space, the probability distribution function of the molecular structure, and the diffusivity of the oil bearing
mineral matter. The overall objective of this subtask is to obtain experimental data that can be used to validate the structural model of kerogen being developed in Subtask 4.6 and to provide data for evaluating kerogen reaction models in Subtask 4.3.

Task Deliverable (Phase II): The Recipient shall submit one paper to a journal such as Energy & Fuel and shall make at least one presentation at a national meeting (e.g., American Chemical Society).

Task 5.0 - Environmental, legal, economic and policy framework

The Recipient shall perform research to address environmental, legal, economic, and policy gaps relevant to in-situ production of oil shale and sands. Research results shall be conveyed through journal articles and public forums and conferences. Task 5.0 shall include the following subtasks:

Subtask 5.1 – Models for addressing cross-jurisdictional resource management

The patchwork of federal, state, tribal and private land ownership that occurs throughout Utah and much of the West creates a range of access, development and management challenges for oil shale/sands development projects. In Phase I, the Recipient shall investigate land ownership and associated jurisdictional issues that may present challenges to the efficient utilization and deployment of in-situ thermal technologies. The Recipient shall also consider issues associated with consolidation of isolated state sections and analyze opportunities for coordinated leasing and regulation of oil shale/sands development units across multiple jurisdictions. Lastly, the Recipient shall address regulatory solutions to these challenges for in-situ thermal oil shale/sands development.

Task Deliverable (Phase I): The Recipient shall generate a Topical Report addressing the land and resource management issues outlined above that shall be submitted to DOE/NETL and at least one article published in a law review or comparable journal.

Subtask Decision Point - Continuation to Phase II activities will be dependent on satisfactory completion of task work and deliverables associated with Phase I efforts as described above, and approved by the NETL Project Officer.

In Phase II, the Recipient shall review the legal requirements regarding access to oil shale and sands resources across federal public lands in the absence of further federal development of these resources. Expanding upon research and analysis conducted under Phase I, the Recipient shall update land and resource ownership quantification estimates following the Utah Recreational Land Exchange Act and seek to identify resource areas with the highest development potential in light of existing resource assessment and development constraints. Lastly, the Recipient shall identify and research models that have been utilized for multi-jurisdictional resource management, conduct case studies as appropriate, and evaluate the utility of these models in the context of oil shale and sands development.
Task Deliverable (Phase II): The Recipient shall generate a Topical Report for DOE/NETL addressing the Phase II land and resource management issues outlined above.

Subtask 5.2 - Conjunctive management of surface & groundwater resources

The overall objective of this subtask is to provide an analysis of water-related issues that shall face developers of unconventional fuels. During Phase I, the Recipient shall seek to identify the environmental policy issues that will likely stem from reassigning water rights as well as the laws that will govern the water quality issues that are anticipated to be relevant in the context of commercial oil shale/sands activities. The focus of this effort shall be on the water resources of Utah. However, due to the complex legal framework, aspects of the study shall encompass the Upper Colorado River Basin. From a legal perspective, the subtask shall outline the state laws that would govern the private purchase of individual water rights, the complex framework of laws that would apply to any potential dam construction, and the federal laws and treaties that govern allocation of Colorado River water resources. From an economic perspective, this subtask shall analyze the potential socio-economic and economic impacts and costs of water reallocation to promote commercial oil shale/sands activities.

This subtask also shall identify and analyze emerging issues stemming from evolving produced water jurisprudence and the utilization of produced water. Produced water, if available for appropriation, represents a potential untapped source of water for commercial energy development. Produced water is normally treated as a waste product and legal requirements focus on disposal rather than acquisition and use. Putting produced water to a beneficial use, however, shall require acquisition of a state water right, raising complex impairment and public interest questions. The Recipient proposes to investigate recent developments in produced water regulation, focusing on produced water regulation within Utah and the legal requirements for using produced water to support in situ thermal processing of oil shale/sands.

Task Deliverable (Phase I): The Recipient shall generate two Topical Reports that shall be submitted to DOE/NETL. The first report shall address the issues and analysis of water availability for oil shale/sands development, and the second report shall address the issues associated with produced water in the context of oil shale/sands development. This subtask shall also generate at least one article published in a law review or comparable journal.

Subtask Decision Point - Continuation to Phase II activities will be dependent on satisfactory completion of task work and deliverables associated with Phase I efforts as described above, and approved by the NETL Project Officer.

For Phase II, the Recipient shall research the current state of conjunctive surface water and groundwater management in Utah, gaps in its regulation, and lessons that can be learned from existing conjunctive water management programs in other states. The Recipient also shall investigate how improved scientific understanding of surface water and groundwater interactions has evolved, how that understanding is, or is not, reflected in Utah’s law regarding the conjunctive management of groundwater resources, and what implications the legal framework for conjunctive management has for oil shale and sands development.
Task Deliverable (Phase II): The Recipient shall generate a Topical Report for DOE/NETL and shall submit an article for publication in a law review or comparable journal addressing issues pertaining to conjunctive water management as described above.

Subtask 5.3 – Policy and economic issues associated with using simulation to assess environmental impacts

The Recipient shall review existing legal issues and constraints relevant to the use of simulation in the context of environmental risk assessment and impacts analysis. The Recipient shall seek to analyze existing legal approaches to various simulation methodologies including (1) distinguishing between traditional statistical predictions and predictions based on established and/or novel simulation science and (2) distinguishing between simulations that do and do not seek to quantify and address uncertainties within the simulations. Additionally, the Recipient shall, analyze the judicial and agency approaches to estimation errors within these varying simulation methodologies and shall examine the economic and environmental policy implications of any erroneous simulation estimations of environmental risks and/or impacts. The purpose of the Recipient’s research is two-fold: (1) to examine how simulation methodologies are commonly assessed in the judicial and agency arena so that simulation scientists can better target areas of concern; and (2) to provide policymakers with analysis of the perceived and practical sufficiency of simulation in the context of environmental risk assessment and impacts analysis.

Task Deliverable (Phase II): The Recipient shall generate a Topical Report for DOE/NETL that assess the legal issues and constraints relevant to the use of simulation in the context of environmental risk assessment and impacts analysis as described above.

6.0 – Economic and policy assessment of domestic unconventional fuels industry

The Recipient shall conduct an assessment that examines limiting factors to the development of domestic heavy oil, oil sands, and oil shale resources and identifies policy, technology, and economic gaps that could be advanced through increased research activities. Subtasks in this research area include:

Subtask 6.1 Engineering process models for economic impact analysis

The Recipient shall provide process models and data to be used in the economic impact analysis conducted in Subtask 6.3. The Recipient shall provide reasonable estimates of construction and operational costs, water utilization, land use and carbon footprint for various in-situ and ex-situ extraction methods, primary and secondary upgrading, refining, and transportation to markets for the following resources:

i. Uinta and Piceance Basin - oil shale
ii. Utah (Uinta and Paradox basins) - oil sands
iii. North Slope area of Alaska - heavy oil
Task Deliverable (Phase I): The Recipient shall provide a Topical Report to DOE/NETL containing a summary of engineering and economic parameters analyzed, a listing of all source data referenced, and a description of the models used. The Recipient shall also upload all models and data to the Institute repository for use by internal and external researchers.

Subtask 6.2 - Policy analysis of the Canadian oil sands experience

The Recipient shall analyze the political and economic similarities and differences between the conditions that facilitated Canadian oil sands development and those that currently exist in the U.S. Initial activities related to this subtask, including the gathering of economic data relevant to assessing whether and how the Canadian oil sands experience is predictive of development of a domestic oil sands industry, were completed in a previous phase of this research. For this subtask, the Recipient shall address the impacts of differences in funding, investment mechanisms and government between the two countries as well as the contrasting market realities facing the oil sands industry in Canada and in the U.S. Additional work in this subtask shall examine the environmental consequences of Canadian oil sands production and emerging post-production environmental management issues, such as rehabilitation of the production sites, wildlife management, air pollution issues, and the scope of tailing pond maintenance, as well as policy issues that have been raised, such as water consumption, the energy in-energy out calculus of oil sands production, and the elevated greenhouse gas emissions that result from bitumen production as compared to conventional oil and gas production. Lastly, the subtask shall seek to place existing and planned oil sands development in Utah in the context of the lessons to be gleaned from the Canadian oil sands model.

Task Deliverable (Phase I): The Recipient shall provide a Topical Report to DOE/NETL describing the results of the policy analysis, its implications for development of U.S. unconventional fuels, and specific lessons that can be gleaned or pitfalls avoided through implementation of the Canadian oil sands model.

Subtask 6.3 – Market Assessment Report

The Recipient shall examine limiting factors to the development of domestic heavy oil, oil sands, and oil shale resources and identifies policy, technology, and economic gaps that could be advanced through increased research activities. This assessment shall emphasize production from three resources: oil shale from the Uinta (Utah) and Piceance (Colorado) Basins, oil sands from Uinta and Paradox Basins (both in Utah), and heavy oil from the North Slope area of Alaska.

The assessment shall use the approach of an economic impact analysis to show likely regional effects from a range of plausible production scenarios. The assessment shall also identify preliminary infrastructure needs that are required for future development of all three resources under various production scenarios (e.g. refining, pipeline, water and power capacity). Additional analysis on the technical and market potential of reducing the carbon footprint of oil sands and oil shale production by considering opportunities for enhanced oil recovery in heavy oil fields shall also be included.
The Recipient shall draw on the technical expertise accumulated by the researchers in Tasks 3.0, 4.0, and 5.0 as well as Subtasks 6.1 and 6.2. For each region, the Recipient shall establish criteria to allow filtering of production scenarios for further study. For example, the induced effects on the commercial viability of a given production scenario due to economic constraints and uncertainties such as the market for refinery outputs, the price of natural gas, and the potential price of CO₂ must be considered. The likelihood and magnitude of these microeconomic impacts shall guide the choice of scenarios because the scenarios get their plausibility from their commercial viability.

The Recipient shall then establish the supply cost for each of these scenarios. Note that the supply cost can be partitioned among construction (amortized), operations, and contingent costs, where contingent costs are those coming from shocks such as rising natural gas, oil, or carbon-emission prices. It is these contingent costs that are most pivotal to viability among the uncertain costs. For each production stage within each scenario, the Recipient shall create lists of construction inputs and of operations inputs. These lists are the feedstock for the economic impact analysis (i.e. the macroeconomic model), which is meant to show the likely regional effects (on employment, income, tax revenue, etc.) from such an operation.

Task Deliverable (Phase I): The Recipient shall provide a draft Market Assessment Report to DOE/NETL for review and a final Market Assessment Report with full graphics layout for public dissemination.

Task 7.0 – Strategic Alliance Reserve (Capstone Project)

The Recipient shall fund collaborative industrial research through a capstone project with American Shale Oil, LLC (AMSO). This project draws together the results of past research to demonstrate computational simulation capability for the assessment and deployment of the shale oil production process commercialized by AMSO. In this integrated project, simulation capability together with experimental data from key small-scale experiments conducted independently by AMSO will be coupled in a formal validation process where the controlling uncertainties are accounted for and quantified. A complete description of this task is included as Appendix A.

Subtask 7.1 – Geomechanical model

The Recipient shall develop non-linear stress-strain relationships for oil shale (or similar materials subjected to in-situ thermal processes) with specific reference to AMSO properties. This constitutive model shall capture the effects of temperature, the in-situ stress tensor, the rate of mechanical or thermal loading on the incremental change in porosity (volume and saturation/infill), tangential values of Young’s moduli, and Poisson’s ratios and post-peak performance. In this research, experimental data are available and these measurements, presumably at different temperatures and stress conditions, shall serve as the basis for developing a constitutive model (i.e. extension of the Duncan-Chang hyperbolic model to transversely isotropic material or similar) that can be applied to numerical modeling of oil shales.

Subtask 7.2 – Kinetic compositional models & thermal reservoir simulators
The subtask has two objectives. The first is to integrate a kinetic compositional model into the Advanced Reactive Transport Simulator (ARTS) such that the efficiency and physical rigor of the reservoir-based simulator more realistically represents the complex processes occurring during oil shale pyrolysis and subsequent production of multiple phases. ARTS is an unstructured grid reservoir simulator for subsurface thermal processes that is capable of incorporating multiple chemical species and chemical reactions. The second is to incorporate the thermal geomechanical constitutive relationships developed in Subtask 7.1 into the current simulator structure. While geomechanics has recently been added to ARTS, the thermal stress aspects have not yet been built in.

Subtask 7.3 – Rubblized bed high performance computing (HPC) simulations

For this task, the Recipient shall use a multiscale, multiphysics, high performance computer (HPC) simulator to compute the behavior of the rubblized bed in the AMSO test by resolving the scale of the individual rubblized pieces of shale. Specifically, the Recipient shall seek to accurately predict the time/temperature history of each piece of shale in a statistical distribution of rubble in the AMSO configuration. The Discrete Element Method (DEM) shall be used to simulate the packing in the rubblized bed such that results are characteristic and provide a geometrical representation of the AMSO test.

Task Deliverables (Phase II): For Task 7 the Recipient shall provide the following:

- Version 1 of the chemical compositional model package
- Generation 1 simulator with V/UQ summary report
- Version 1 of the geomechanical model with report
- Topical report on ARTS and conventional reservoir simulation results with rigorous kinetics and poroelastic changes
- Generation 2 simulator with V/UQ summary report
- Topical report on integrated thermal simulations with geomechanics of the AMSO geometry/conditions using both ARTS and conventional reservoir simulator
- Final project report

D. DELIVERABLES

The Recipient shall provide reports in accordance with the enclosed Federal Assistance Reporting Checklist and the instructions accompanying the Checklist. In addition to the reports identified on the Reporting Checklist, the Recipient shall provide the following:

- Project Management Plan
- Topical Reports submitted through OSTI
- Presentations and/or papers presented at technical conferences
- Peer-reviewed technical papers written and submitted to archival journals
- Law review articles
• Papers distributed through the Recipient’s online repository after an internal review process

E. BRIEFINGS

The Recipient shall prepare detailed briefings for presentation to the Project Officer at the Project Officer’s facility located in Pittsburgh, PA or Morgantown, WV. Briefings shall be given by the Recipient to explain the plans, progress, and results of the technical effort on an annual basis. DOE may substitute attendance of meetings at NETL with Recipient participation in external project/merit reviews. In addition, NETL shall be advised a priori of paper submissions and of conference presentations.

ADDENDIX A – Statement of Program Objectives for Strategic Alliance Reserve
Background

Unconventional fuels research, specifically oil shale and oil sands, has a history at the University of Utah that dates back to the 1970s with seminal work performed by Professors HY Sohn, JD Miller, FV Hanson, Dr. James Bunger, and others. Renewed interest in the potential development of Utah’s oil shale and oil sands resources led to the formation of the Utah Heavy Oil Program (UHOP) within the Institute for Clean and Secure Energy (ICSE) in 2006. The mission of UHOP was to provide research support to federal and state constituents for addressing the wide-ranging issues surrounding the creation of an industry for oil shale, oil sands and heavy oil production in the United States. UHOP was broad and interdisciplinary in nature with faculty participants from the Colleges of Engineering, Mines, Law, Business, and Science. Research projects included a detailed geological analysis of an oil shale well coupled to reservoir modeling that accounted for the geological heterogeneity, an evaluation of potential in-situ production methods from a representative Utah oil sand formation, data collection for the development of a detailed kinetic model of oil shale pyrolysis, a study on water demand for commercial oil shale development and potential treatment systems for produced water, and the identification of environmental, policy, economic and socioeconomic issues relevant to determining when and how a federal commercial oil shale program might be implemented. This research was complemented by the release in 2007 of “A Technical, Economic, and Legal Assessment of North American Heavy Oil, Oil Sands, and Oil Shale Resources.”

Beginning in 2009, the program was renamed the Clean and Secure Energy from Domestic Oil Shale and Oil Sands Resources Program to better represent the research that was being conducted. The new Program retained the multidisciplinary nature of UHOP and began actively seeking opportunities to work with industry and with state and federal governments to deliver research results that would have an immediate impact. Collaborations were established with the Utah Geological Survey, Red Leaf Resources, Argonne National Laboratory, and the Utah Bureau for Economic and Business Research. Research projects were focused in four primary areas: (1) oil shale/sands utilization with efficient CO₂ capture through the introduction of oxy-fuel process heaters to produce a high concentration CO₂ stream that is sequestration-ready, (2) creation of models and simulation tools for application to in-situ thermal processing of oil shale/sands, (3) analysis of legal, policy and economic gaps that pertain to in-situ liquid fuel production from oil shale/sands, and (4) the preparation and publication of a market assessment that analyzes the supply costs and economic impact of various oil shale/sands development scenarios in Utah’s Uinta Basin. An additional research area was added in FY2010 that is focused on the development of a predictive tool for assessing the basin- or regional-scale environmental and economic impacts of unconventional fuel production. In all research areas, a strong emphasis has been placed on integrating information from a range of scales and on using appropriately validated tools to facilitate the rapid dissemination of technology.

This capstone project is intended to draw together the results of these past many years of research to demonstrate computational simulation capability for the assessment and deployment of the shale oil production process commercialized by American Shale Oil, LLC (AMSO). In this integrated project we couple this simulation capability together with experimental data from key small scale experiments conducted independently by AMSO in a formal validation process where the controlling uncertainties are accounted for and quantified. It is our thesis that the optimal risk assessment and decision-making regarding deployment of this new technology can most efficiently be accomplished by this formal simulation - validation and uncertainty quantification process.
1. Geomechanical Model

This task will be led by Professor John McLennan.

OBJECTIVE

This research proposes the development of non-linear stress-strain relationships for oil shale (or similar materials subjected to in-situ thermal processes) with specific reference to AMSO properties. This constitutive model will need to capture the effects of temperature, the in-situ stress tensor, and the rate of mechanical or thermal loading on the incremental change in porosity (volume and saturation/infill), tangential values of Young’s moduli, and Poisson’s ratios and post-peak performance.

Oil shales such as the Green River Shale or Mahogany Shale are laminated, kerogen-rich, fine grained anisotropic (or at a minimum transversely isotropic) rocks whose properties are heavily controlled by temperature. AMSO’s engineered thermal treatments will affect the in-situ stress conditions (there can be thermally-dependent coefficients of thermal expansion), pore pressure (the proposers are even uncertain of the applicability of effective stress concepts for these materials), porosity and permeability (superficially one would anticipate an increase, although compactive behavior cannot be ruled out). The process will also alter local incremental deformation and load bearing characteristics. The medium’s behavior, therefore, is non-linear, stress-dependent, temperature-dependent, and time-dependent, and possibly rate-dependent.

It is anticipated that the constitutive relationships would be adaptable for use in commercial third party numerical simulators run by others, Agapito for example. In this work, experimental data are available and these measurements - presumably at different temperatures and stress conditions will serve as the basis for developing a constitutive model (i.e. extension of Duncan-Chang\(^1\) hyperbolic model to transversely isotropic material or similar) that can be applied to numerical modeling of oil shales.

STATEMENT OF WORK

The tasks are:

- **TASK 1.1**: Gather all available data including stress-strain curves, creep data, and associated basic rock properties (porosity, permeability, mineral composition, TOC, \(E\), \(\nu\), etc.) of oil shales, especially at elevated temperatures. There are some limited data in the public domain\(^2\),\(^3\),\(^4\) that could supplement the information already generated by AMSO.
- **TASK 1.2**: Briefly survey the key publicly available constitutive relationships used in commercial simulators. Some of these will be modified from relationships that are used for unconsolidated geomechanical materials (for example, Duncan and Chang, Vaziri and Byrne,\(^5\) Brown et al.,\(^6\) Ciz and Shapiro\(^7\))
- **TASK 1.3**: Develop a process for multivariate delineation of material behavior in at least three parameters (a set of surfaces in deviatoric stress, axial and radial strain and temperature, the surfaces varying with confining pressure and possibly thermal history).

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\(^2\) Budd, C. H., McLamore, R. T., and K. E. Gray, 1967, Microscopic Examination of Mechanically Deformed Oil Shale, SPE paper 1826.
• **TASK 1.4:** Attempt to infer permeability-porosity-temperature relationships. This is an extremely difficult task. Most historic Kozeny-Carmen representations have bogged down in comprehending tortuosity. All that can be realistically committed to is compiling and evaluating any available data.

• **TASK 1.5:** Test relationships in relevant software including MPM in Uintah and appropriate commercially available continuum or discrete element thermal-poro-hydro-mechanical simulators. In particular, for University of Utah calculational programs ensure that the appropriate constitutive models are available for use in any coupled or independent codes.

• **TASK 1.6:** Interact with teams carrying out the other tasks in this effort.

• **TASK 1.7:** Suggest experimental data that would be relevant.

### 2. Kinetic Compositional Models & Thermal Reservoir Simulators

*This task will be led by Professor Milind Deo.*

**OBJECTIVE**

The objective of this task is to package the kinetic compositional model so that it can be incorporated into simulators at the University of Utah (and elsewhere) and to enhance the efficiency and physical rigor of the the reservoir-based simulator to more realistically represent all the complex processes during oil shale pyrolysis and subsequent production of multiple phases.

Over the last few years, we have developed an unstructured grid reservoir simulator for subsurface thermal processes called ARTS (Advanced Reactive Transport Simulator). This is a K-value based thermal reservoir simulator capable of incorporating multiple chemical species and chemical reactions. It uses natural variables (saturations, pressures and temperatures). The formulation is fully implicit and analytical Jacobian is used in the solution\(^8\). The simulator was validated by using data available on in-situ combustion laboratory adiabatic combustion tube experiments\(^9\). The temperature profile after six hours in the combustion tube is shown in Figure 1.

![Figure 1: Experimental and simulated temperature profiles for the Smith and Perkins adiabatic combustion tube experiment. Agreement between the experiment and the model is reasonable considering that the components, stoichiometry and rates proposed in the experimental study were used without any modifications.](image)

Geomechanics has recently been added to The University of Utah reservoir simulator framework. The current structure of the simulator is shown in Figure 2.

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The geomechanical constitutive equations currently in place in ARTS do not have the thermal stress aspects built in. The general formulation of the geomechanical module both in the discretization and the physical model components of the program will allow incorporation of the thermal geomechanical constitutive relationship (to be explored in Task 1).

**STATEMENT OF WORK**

The tasks are to use ARTS and/or conventional reservoir simulators to:

- **TASK 2.1:** Simulate the slanted well geometry being examined in AMSO’s pilot process.
- **TASK 2.2:** Package the chemical component, stoichiometric and kinetic models for incorporation into thermal reservoir simulators and the high resolution rubblized bed Simulators of Task 3.
- **TASK 2.3:** Investigate the porosity-permeability evolution as the temperature front moves away from the heater well by conduction and by convection.
- **TASK 2.4:** Consider the re-condensation and reflux of the heavier components.
- **TASK 2.5:** Study the production of liquids and condensable vapors from the wells.

The thermal geomechanical aspects will be examined first (without flow) in the simulator prior to integration with flow components of the simulator.

3. Rubblized Bed HPC Simulations

*This task will be led by Professor Philip Smith.*

**OBJECTIVE**

The research that we have conducted at ICSE over the past five years has shown that:

- Heat transfer through the shale bed is the rate limiting process for production of shale oil (i.e. not thermal decomposition of kerogen, mass transfer from the mineral matrix, etc.).
- Convective heating in a rubblized bed of shale reduces the time for the shale bed to reach shale oil production temperature over conductive heating in the bed.
- High performance computing (HPC) can be used to simulate rubblized bed convective heating for oil shale by resolving the scale of individual channels and shale pieces.

For this task we propose to use a multiscale, multiphysics, high performance computer simulator to compute the behavior of the rubblized bed in the AMSO test by resolving the scale of the individual rubblized pieces of shale. Specifically, we are seeking to accurately predict the time...
temperature history of each piece of shale in a statistical distribution of rubble in the AMSO configuration. The system to be solved is schematically represented in Figure 3.

From Task 1 we will obtain a model that will give insight into a characteristic distribution of thermally fractured particles that constitutes the rubblized bed. The packing in this bed will be simulated with a Discrete Element Method (DEM) that results in a characteristic geometrical representation of the AMSO test. The hot gases/liquids from the region of the heater will result in a natural circulation that convectively heats the surface of individual pieces of shale in the bed. The fluid mechanics of the natural convection will be computed through all of the individual channels in the bed. Conductive heating of the individual pieces of shale from the surface to the center is simultaneously computed. Thus, the time-temperature history of each and every piece of shale will be computed in the simulation. Required thermal properties of the shale pieces will be acquired from research in Task 1 and from AMSO.

Figure 3: A schematic representation of an integrated simulation of the AMSO test wells.
A model for the yield of gas and liquid products as a function of temperature will be incorporated into the simulation by drawing on the research of Task 2 and the models available from AMSO.

**STATEMENT OF WORK**

The tasks are:

- **TASK 3.1:** Knowledge Collection - Collect AMSO background knowledge and data about the characteristics about the operation of the heated wells. This will include any known information about:
  - the geometry of the bed and its evolution over time as the formation is heated,
  - thermal properties of the shale,
  - operating conditions,
  - product yield models as a function of temperature,
  - physical and chemical characteristics of the shale.

- **TASK 3.2:** Generation 1 Simulation - Perform DEM, CFD and Thermal analysis of a characteristic section of the AMSO rubblized bed. This base case simulation will be built from the knowledge base acquired in Task 3.1 and the research accomplished under Task 1 of this research project. It will incorporate a simple thermal response model for the product yields (i.e., product yield as a function of shale temperature). The results of this task will be the first generation prediction of the production rates from the AMSO process. The resulting integration of these models that produces this base case simulation will become a product of this research and delivered to AMSO.

- **TASK 3.3:** V/UQ of Gen 1 Sim with AMSO Expt. Data - Experimental data collected from the AMSO tests will be used in conjunction with the Gen 1 Simulator of Task 3.2 to produce a formal validation / uncertainty quantification (V/UQ) for the predictivity of the Gen 1 Simulator. This uncertainty quantification will include quantified uncertainties in the most important scenario parameters, model parameters, numerical parameters and experimental data.

- **TASK 3.4:** Generation 2 Simulation - Incorporate the kinetic compositional models of Task 2 as they become available and/or include such models from AMSO as collected in Task 3.1. This becomes the Gen 2 Simulator. Perform fully coupled DEM, CFD, Thermal and Chemical simulation of a characteristic section of the AMSO rubblized bed. The resulting integration of these models that produces this base case simulation will become the second generation product of this research and delivered to AMSO.

- **TASK 3.5:** V/UQ of Gen 2 Sim with AMSO Expt. Data - Ongoing experimental data collected from the AMSO tests will be used in conjunction with the Gen 2 Simulator of Task 3.4 to produce a formal validation / uncertainty quantification for the predictivity of the Gen 2 Simulator. This uncertainty quantification will move beyond the V/UQ of Task 3.3 by building on the lessons learned from that task.

4. **Budget**

This two year project will be funded by The Department of Energy, with AMSO contributing experimental data, models for chemical processes, advice and direction on the project. Meetings will be held every four months with AMSO (or more often as needed) to give appropriate feedback and direction to the project. The budget breakdown is shown in the following table.
5. Project Management

A Gant Chart with milestones is shown below for this project.

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<th>DOE/UU Funding (2 yrs)</th>
<th>TASK 1 - McLennan</th>
<th>TASK 2 - Deo</th>
<th>TASK 3 - Smith</th>
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</tr>
</tbody>
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6. Deliverables

The project deliverables are:

• 9 mo. - Version 1 chemical compositional model package

• 12 mo. - Gen 1 simulator with V/UQ summary report.
  ▸ Topical report on ARTS and conventional reservoir simulation results with rigorous kinetics and poroelastic changes.
  ▸ Version 1 of the geomechanical model with report.

• 24 mo. - Gen 2 simulator with V/UQ summary report.
  ▸ Topical report on ARTS and conventional reservoir simulator integrated thermal simulation results with geomechanics of the AMSO geometry and conditions.
  ▸ Final Report of Project