ATTACHMENT 3 – STATEMENT OF PROJECT OBJECTIVES

CLEAN AND SECURE ENERGY
FROM COAL, OIL SHALE & OIL SANDS

A. OBJECTIVES

The University of Utah (the Recipient), via their Institute for Clean and Secure Energy, shall pursue interdisciplinary, cradle-to-grave research and development of energy for electric power generation and for liquid transportation fuels from the abundant domestic resources of coal, oil sands, and oil shale. Emphasis will be on minimizing the environmental impacts associated with the development of these resources, including reducing the carbon footprint through the use of CO_2 capture for subsequent storage (sequestration).

General project objectives include developing and completing tasks that advance the framework within which coal, oil shale and oil sands resources are being developed; using project research, analysis and conclusions to identify missing elements (technical, legal, economic and policy) that will be necessary for future development of these resources; and gathering and making available a wide range of information relevant to development of these resources that can aid policy makers and other researchers and analysts. Specific project objectives include:

Clean Coal Program – The objectives of the four program thrust areas are as follows:

- Oxy-Coal Combustion Thrust Area – To address engineering and computational questions that surround the design and operation of oxygen-fired combustion systems, with particular emphasis on minimizing costs and technical problems associated with flue gas recycle.

- High-Pressure, Entrained-Flow Coal Gasification Thrust Area – To 1) develop quantified predictive simulation tools for high pressure entrained flow gasifiers, 2) acquire fundamental data to fill gaps in the understanding of coal conversion under high pressure gasification conditions, 3) develop computational models for the simulation tools and (4) acquire data from operating gasifiers for simulation and model validation.

- Chemical Looping Combustion Reactions and Systems Thrust Area – To 1) provide a mechanistic understanding and chemical reaction rates for copper metal/copper oxides and 2) conduct process modeling and preliminary economic studies to provide a basis for improvement in the future.

- Sequestration Thrust Area – To study the impact of contaminant gases on sequestration chemistry, with a particular focus on the assessment of the risk of CO_2 leakage.

Oil Sands and Shale Program –The primary objective of the Oil Sands and Shale program is to understand the fundamental technical processes underlying the development, production, and utilization of these resources in an environmentally responsible manner.

Policy, Environment, and Economics Program – The primary objective of this program is to evaluate numerous policy, legal, environmental, and economic issues raised by ongoing coal, oil shale, and oil sands development to facilitate and aid in the rational development and utilization of these resources.

B. SCOPE OF PROJECT

The Recipient shall perform a range of academic research tasks addressing issues common to classes of energy processes and multiple energy technologies, rather than addressing company-specific and potentially proprietary processes. The Recipient shall:

- Conduct a set of tasks that builds from the strengths of the institute to provide open (non-proprietary) results on the development, production and utilization of coal, oil shale and oil sands for both power generation and liquid transportation fuels in a carbon-constrained world.

- Prepare and disseminate updated technical, legal, and economic assessments through reports, papers, workshops, and an online repository on the domestic development, production and utilization of coal, oil shale, and oil sands; and bring together industry, government and the public for analyzing energy options, policy and implications.

- Develop and validate modeling and simulation tools for reducing and eliminating greenhouse gas emissions from power generation and liquid transportation fuel production drawing from expertise in high performance computing, and multi-physics, multi-scale modeling.

To produce predictive quantification of energy options requires formal verification and validation processes that rely on consistency between experimental observations and simulation results to make predictions and quantify uncertainty. Consequently, the Recipient shall organize this project around the principle of validation, integrating a consistent and systematic interpretation of experiments, models and simulations to:

- Explain the experimental and simulation data sets together in order to quantify the ranges of behavior exhibited by both.

- Quantify uncertainty and communicate the sensitivities and sources of uncertainty in ways that are accessible to both policy makers and technology decision makers.

- Incorporate the legal, policy and socio-economic factors that influence final outcomes.

C. TASKS TO BE PERFORMED

Specific tasks are organized into a Management area and three Program areas – the Clean Coal Program, the Oil Shale and Sands Program, and the Policy, Environment, and Economics Program.

MANAGEMENT

Task 1.0 – Project Management

<u>Subtask 1.1 – Project Management and Planning</u>

The Recipient shall finalize the Project Management Plan within 30 days after award and manage project activities in accordance with the plan. The Project Management Plan will be updated as necessary.

Subtask 1.2 – Briefings and Reports

The Recipient shall monitor and coordinate the technical and financial activities of the project and will prepare and deliver reports and briefings as outlined in Sections D and E below.

Task 2.0 - Industrial Advisory Board

The Recipient shall create an industrial advisory board to provide input in the selection of Institute-sponsored tasks/projects and, together with DOE, provide annual review of ongoing tasks/projects. The board will be finalized by November 2008 and convene in March 2009. Currently funded tasks shall be required to provide task status reports to the board prior to the March 2009 meeting.

Task 3.0 - Student Research Experience at DOE NETL

The Recipient shall work closely with their NETL points of contact to offer select graduate and undergraduate research opportunities at NETL. The duration of a graduate research experience is expected to last from 4 months to one year while the undergraduate experience is expected to last one summer. The Recipient shall recruit students at the University of Utah to participate in this program.

CLEAN COAL PROGRAM

The tasks for the Clean Coal Program are organized into four thrust areas: Oxy-Coal Combustion, Gasification, Chemical Looping Combustion, and Carbon Sequestration.

Oxy-Coal Combustion Thrust Area

Oxy-Coal Combustion is a promising, low-cost technology applicable for global implementation of new energy systems as well as for retrofitting traditional boilers and furnaces. It enables CO_2 capture by direct compression of flue gas for immediate transportation and sequestration. However, the operation and performance of the combustion chamber requires that some of the flue gas be recycled to maintain design temperatures and operating conditions. A multitude of scientific, engineering and computational questions surround the design and operation of existing and new combustion systems under oxygen firing. The following tasks will begin to address these questions using simulation as the vehicle for integration and innovation.

Task 4.0 – Oxy-Coal Combustion Large Eddy Simulations

In this task, the Recipient shall continue the development of a new computational fluid dynamics (CFD) tool for exploring the near-burner region of an oxy-coal flame. In an effort to predict important aspects of the oxy-coal flame that were previously unpredictable, we are using a Large Eddy Simulation (LES) method for the evolution of the turbulent jet and a moment method to represent the coal phase particle behavior. This development effort will use the data obtained in Tasks 5.0 and 6.0 (below) to achieve quantifiable predictivity with uncertainty bounds by closely coupling the experimental data with the simulation. The Recipient shall collaborate with NETL in-house researchers, scientists and program offices to ensure that the efforts proposed and implemented are complementary to the large body of past and ongoing work conducted at NETL.

During previous Utah Clean Coal Program efforts, researchers developed the verified LES algorithm and framework and demonstrated the feasibility of moment methods for particle descriptions in LES. Using concepts of one-dimensional turbulence (ODT), sub-grid scale models for the particle were initiated and established two-step and distributed activation energy models for devolatilization reactions were incorporated. An oxy-coal validation hierarchy was established in conjunction with the experimental program. This work was built on the LES tool, ARCHES, a massively parallel, variable density, finite-volume code developed under DOE-ASC funding for fire applications.

This task specifically focuses on validating computational results of the near-burner region in oxy-coal combustors. Using ARCHES, the Recipient shall investigate three critical questions with the coupled simulation and experimental data: 1) Can we predict particle distribution changes in the near-burner region? 2) Can we predict ignition/kinetic/aerodynamic interactions in the near-burner region? 3) Can we produce quantifiable uncertainty bounds on our predictions?

The Recipient shall investigate these questions by:

- Expanding the moment method for the particle phase description to include multiple internal coordinates for the particle distribution function. Specifically, internal coordinates will be included for: (1) particle size (already included), (2) particle velocity (previous LES work assumed the particles and gases moved at the same velocity), and (3) particle composition.

- Continuing the particle-phase ODT model for sub-grid particle descriptions and source term closure. Specifically, manifolds will be extracted from the ODT model for application to the pilot-scale simulations. The error budget for including different sub grid models will be quantified.

- Continuing validation efforts using the hierarchy developed under the previous research by performing uncertainty quantification on the University of Utah reactor being probed under tasks 5.0 and 6.0.

Task 5.0 – Experimental Studies of Oxy-Coal Combustion

This task will focus on developing enabling technologies for oxy-coal combustion and will build upon the capabilities developed previously under the Utah Clean Coal Program via three subtasks.

<u>Subtask 5.1 – Near-Field Aerodynamics of Oxy-Coal Flames with Directed Oxygen and Minimum Flue Gas Recycle</u>

This subtask provides insight into how directed oxygen injection can be employed to make oxy-coal combustion more economical by minimizing costs and technical problems associated with recycling more than four times the resultant exhaust gas. Subtask objectives include:

- Developing fundamental strategies for *directed* O_2 injection with minimum CO_2 recycle in oxy-coal flames.

- Providing validation data for near field aerodynamic simulations of well defined oxy-coal flames with non-uniform injection of O_2 and minimum CO_2 recycle.

- Educating at least one Ph.D. graduate student for research in the oxy-coal combustion field.

Large amounts of recycle are currently planned for first generation oxy-coal processes where the equipment closely resembles existing boilers as far as heat transfer is concerned. This subtask provides the science behind enabling technologies not only for those first generation processes but also for second-generation oxy-coal processes, where directed streams of pure oxygen allow recycle to be minimized without radical boiler redesigns. Specifically, the research will address the following questions: 1) How should pure O_2 be injected into the furnace? 2) What is the minimum CO_2 flow required for the fuel jet (or for other streams)? 3) How should O_2 and CO_2 flows be distributed if CO_2 is required? 4) What are heat fluxes to furnace walls under these conditions? 5) What are the flame shapes and characteristics? 6) What are the temperature, gas composition, particle size, and particle and gas velocity fields as measured through newly developed diagnostics (longer-term activity)? 7) What coal particle ignition, pyrolysis and oxidation mechanisms must be considered to allow for model development of these configurations?

For this subtask, the Recipient shall modify the existing oxy-fuel combustor by replacing the heated walls with water-cooled walls in the furnace top section. This modification will allow maximum local flame temperatures without material degradation and will permit the quantification of average heat fluxes. For an initial configuration, the Recipient shall build on existing work on axial coal jets. The coal will be transported by pure CO_2 and the initial flow of oxygen will be injected axially into the center of the coal jet such that the unburned coal particles shield the walls from excessive heat fluxes. A secondary axial flow of CO_2 and O_2 will surround the two interior jets and will be adjusted for minimum CO_2 entry into the furnace, consistent with survival of the cooled furnace walls. Measurements will consist of inlet and outlet temperatures of cooling water for the water walls (average heat flux), and instantaneous electronic photographic records of flame shape and flame length as well as spatially and temporally resolved data from more advanced diagnostics (see Task 6.0).

This subtask will produce validation data for simulations of near-field flame aerodynamics with multiple inlet oxidant streams. This simulation capability developed by integrating Task 5.1 and Task 4.0 will play a critical role in guiding second generation oxy-coal combustion technologies toward optimum (or possibly minimum) flue gas recycle ratios, both for retrofit applications and also for new units.

<u>Subtask 5.2 – Ash Partitioning Mechanisms for Oxy-Coal Combustion with Varied Amounts of Flue Gas Recycle</u>

This subtask will provide critical information for the development of ash deposition sub-models for oxy-coal combustion with both large and minimal (using directed O_2 injection, for example) amounts of flue gas recycle. Subtask objectives include:

- Determining the effect of varied amounts of flue gas recycle on ash partitioning mechanisms.

- Providing validation data for sub-models predicting size-segregated ash particle composition as a function of the environment in oxy-coal flames with flue gas recycle amounts ranging from 0-30%.

- Educating at least 2 Ph.D. students for research in ash particulate formation and oxy-coal combustion processes.

Ash deposition, which controls convective heat transfer to superheater tubes, depends on mechanisms of ash partitioning that are determined by the local temperatures and gas compositions through which the coal particles travel. This subtask will uncover the critical ash partitioning mechanisms and determine the optimum flue gas recycle configuration from an ash deposition and fouling point of view. Specifically, the research will be conducted on two scales: 1) externally heated drop-tube studies involving micro-flows (~1-4 g/h) of coal particles, and 2) tests on existing oxy-fuel combustor (OFC) involving self-sustained combustion and coal flows of ~10kg/h.

The drop-tube studies and the OFC studies are complementary. The drop-tube studies use *simulated* recycled flue gases while the OFC studies use actual recycled flues gases. The drop-tube studies will focus on well-defined tests in which temperature and local surrounding gas compositions are systematically varied to allow a wide range of ash formation environments. Total exhaust particulate samples will be size segregated using low pressure impactors, and the evolution of the ultra-fine ash particle size distribution will be determined using scanning electron mobility particle sizing techniques. More sophisticated ash analyses will be conducted as warranted. The objective of these tests is to determine how gas composition, O_2 concentration and wall temperature affect the composition and particle size distribution of the ash. These data will form the basis of sub-models that will be tested in the larger scale OFC experiments. The OFC tests will use the modified combustor described in subtask 5.1. In addition, a flue gas recycle system will be installed. Flue gas recycle (FGR) is critical as it produces a more realistic composition of the gas mixture (in terms of O_2, SO_2, NO, and recycled ultra-fine particles), which may control mechanisms of ash partitioning in the field. Tests on the OFC will be conducted with varying amounts of FGR, including tests with minimum or zero FGR that use directed O_2 injection into the furnace. This latter configuration leads to a range of local environments in which ash is formed and is related to the more homogeneous kinetic drop-tube data through sub-models that incorporate mixing. Both drop tube and OFC research will be coordinated with related international and national research efforts under existing collaborative arrangements between the PIs and research institutions in Australia, China, Europe and the U.S. These collaborative arrangements are available at no cost to the project.

The subtask will provide validated ash partitioning sub-models that will be integrated into simulations of the overall oxy-coal combustion process as described in Task 4.0. This simulation capability will provide guidance in both retrofit and new applications of oxy-coal combustion with the end product focused on minimizing the carbon footprint of coal combustion systems at minimum cost.

Subtask 5.3 - Oxy-Coal Combustion in Circulating Fluidized Beds

The Oxy-Coal Team will identify optimal operating conditions for oxy-coal combustion in Circulating Fluidized Beds (CFBs) and will simultaneously produce detailed model validation data for the DOE/NETL MFIX code. While the bulk of oxy-coal applications will be in pulverized coal (PC) fired units, some low-quality coals would be more amenable to firing in a CFB due to the opportunity for significantly increased solids residence time. In addition, oxy-coal firing in a CFB provides an additional degree of freedom over PC firing due to the external recycle of solids back into the combustor.

The recently modified CFB will be used to study the impact of external heat removal from the solids recycle stream on the performance of the CFB, with a specific emphasis on varying the level of CO_2 recycle required for satisfactory performance. Detailed mapping of temperature, species concentrations and particle concentrations will be made under limited conditions for use by DOE/NETL computational staff in their validation efforts of the MFIX model for fluidized bed combustion. Particle concentrations will be measured using an acoustic probe that has shown promise for distinguishing local particle concentrations in preliminary studies. The probe will be further developed under this program for application to combustion conditions. The impact of CO_2 recycle on nitrogen release from coal char will continue to be explored. Additional work on issues relating to the effects of CO_2 on in-bed sulfur capture will also be explored, such that mechanisms can be proposed and corresponding rates quantified for eventual use in simulations of NO_x and SO_x emissions under oxy-coal firing conditions.

Task 6.0 – Advanced Diagnostics for Oxy-Coal Combustion

The Advanced Diagnostics Team will develop advanced diagnostic capabilities for use in oxy-coal combustion experiments that will provide high-fidelity data for the validation of oxy-coal simulation models. Specifically, the Team plans to adapt Particle Image Velocimetry (PIV) for identification of velocity fields in turbulent oxy-coal flames. The application of this method will be done in stages in the laboratory by scaling from relatively simple to more complex systems. Initial efforts will utilize a simple laboratory diffusion flame with gaseous fuel to ensure the methodology has been properly implemented and that all necessary data and image processing techniques have been fully developed. Data from this diffusion flame will be compared with results from other laboratories. Success at this stage of development will lead to application of the diagnostics for the oxy-fuel combustor (OFC), which was specifically designed for the generation of model validation data with turbulent oxy-coal flames. The OFC design includes four-quadrant optical access in the main burner zone to allow application of laser-based diagnostics.

The approach outlined for scaling the diagnostic methodology will also provide data for model validation at different scales and at increasing levels of experimental complexity to aid in the hierarchical nature of the verification and validation/uncertainty quantification (V&V/UQ) strategy.

Task 7.0 - Fate and Control of Mercury in Coal-based Power Generation Systems with CO_2 Capture

The Mercury Team will explore various options for controlling mercury emissions for oxy-coal combustion and for integrated gasification combined cycle (IGCC) units. Mercury capture at high temperatures (> 1000°C) in gasification units is problematic because carbon-based adsorbents are ineffective at high temperatures and can be gasified, and mineral-based adsorbents appear to be ineffective under high temperature, reducing conditions. Mercuric sulfide sublimes at 600°C and 1 atm. It is possible that mercuric sulfide is stable at the high pressures (40 atm) found in gasification processes. No other known mercury compounds are stable at the elevated temperatures and reducing conditions found in gasification units.

The effect of high CO_2 concentrations on the kinetics of homogeneous and heterogeneous oxidation of mercury by halogens will be explored in two simulation-based studies:

- CHEMKIN, a commercially available software tool for solving complex chemical kinetics problems, will be used to study homogeneous oxidation kinetics.

- University of Utah software (developed under the current Utah Clean Coal Program) will be used to study heterogeneous oxidation with adsorption and oxidation kinetics. Kinetic parameters from a variety of sources will be considered.

The Mercury Team will perform simulations of homogeneous oxidation kinetics at temperatures ranging from 250-1000°C and quench rates of 200-450°C/s. The heterogeneous calculations will be performed at 125°C. Both calculations will assume a composition of 90% CO_2, 10 $\mu g/m^3$ Hg, 100 ppm chlorine, and 10 ppm NO_2. In addition, the thermodynamics of HgS at gasifier conditions will be examined to determine whether further study is warranted. This task will build upon the models developed under the current Utah Clean Coal Program.

High Pressure, Entrained-Flow Coal Gasification Thrust Area

Gasification of coal offers several advantages over conventional coal combustion technology, including higher overall energy efficiency, the flexibility of syngas usage (power production via IGCC or catalytic fuel production) and the opportunity to capture generated CO_2 for sequestration. Consequently, interest in coal gasification has increased dramatically in recent years, and once it is clear what the U.S. policy on CO_2 will be, it is expected that several new coal gasification projects will be announced.

The Clean Coal Program is actively researching entrained-flow coal gasification and has several projects in this area. The overall objectives are: 1) to develop quantified predictive simulation tools for high pressure entrained flow gasifiers, 2) to acquire fundamental data to fill gaps in the understanding of coal conversion under high pressure gasification conditions, 3) to develop computational models for the simulation tools and (4) to acquire data from operating gasifiers for simulation and model validation.

The following tasks in this thrust area will address these objectives.

Task 8.0 - Entrained-Flow Coal Gasifier Simulation and Modeling

Science-based simulations are poised to deliver quantifiable predictive performance to a wide range of societal problems. Coal gasification with carbon capture is one of these grand challenge problems. The long-term objective of this task is to integrate modeling components developed by the experimental gasification observations being made within the Clean Coal Program (Tasks 9.0-12.0) with the LES coal simulation capability being developed for oxy-coal combustion (Task 4.0) to produce a high-pressure, entrained-flow gasification simulation tool for scale-up, problem solving, and design of coal gasifiers. The LES tool will be coupled with the experimental data being obtained under this program to provide V&V/UQ. The ultimate goals are: 1) to develop the LES gasification tool, 2) to provide accurate sub-grid scale models applicable to gasification simulation, and 3) to provide quantitative and reliable uncertainty bounds on LES gasification predictions.

Subtask 8.1 - Large Eddy Simulation (LES) of UofU Entrained Flow Gasifier

The Recipient proposes to use the oxy-coal LES simulation tool being developed under Task 4.0 as a foundation in which to incorporate the particle and ash models and mechanisms identified under Tasks 10.0, 11.0 and 12.0 for entrained flow gasifiers. The Recipient shall incorporate these same particle and ash models into the ODT sub-grid models being developed for the oxy-coal system (Task 4.0). These models will become the basis for the sub-grid elements of the LES entrained flow gasifier simulator. These methods will draw on the moment methods (QMOM, DQMOM) under development. To the knowledge of these authors, no LES simulation of entrained flow gasification has ever been performed. This research effort will produce a new level of fidelity of gasification simulation technology never yet demonstrated. The Recipient shall generate simulation results that are coupled with experimental results to produce results with quantified error bars.

Producing quantifiable answers to the questions posed by society about gasification systems depends on being able to put reliable error bounds on the results of large-scale simulations. In such simulations, many sources of uncertainty exist, including parameters in governing equations, boundary conditions, simplifications to physical models, and approximations in numerical methods. Validation/uncertainty quantification (V/UQ) of the gasification simulations will be an integral part of the gasification simulation and application effort. This subtask will include an assessment of the potential variability of a simulation model's computed output given inaccuracies in both the model and in the experimental data.

Subtask 8.2 - Sub-Grid Scale Models

Multi-scale simulations in coal combustion, in gasification and in oil shale/sands processing require hierarchical models to address the nonlinear coupling across the multitude of length and time scales, many of which remain unresolved. It is widely recognized that low-dimensional attractive manifolds exist within these multi-scale systems. The effect of such manifolds is to produce correlations in state variables (e.g. temperature and composition). Direct Numerical Simulation (DNS) remains the most detailed method to analyze turbulence-chemistry interactions, and hence the manifestation of manifolds in the thermochemical state. Under this subtask, Principal Component Analysis (PCA) will be used to identify correlations among state variables in reacting flow systems using DNS data. PCA provides a rigorous and systematic methodology to construct reduced models from large data sets (e.g. DNS data).

In addition, this subtask will extend previous validation efforts of ODT for nonreacting flow to reacting flow using high-fidelity DNS datasets for syngas oxidation. The ODT model (see Task 4.0) has been proposed as a low-cost methodology to approximate the statistics obtained from DNS. This extension will provide validation that is relevant to gasification, oxy-coal combustion, and oil shale/sands processing. The ODT model will employ the detailed kinetics and transport used in the DNS calculations. Additional DNS calculations will be performed for gasification, oxy-fuel combustion, and oil shale/sands systems to validate the ODT model in that context as well. Validation of the ODT model using moderately simple chemistry is a critical step in validating the ODT model for coal combustion. This validation will be done in conjunction with ongoing efforts to develop and validate the ODT model for particle-laden flows, with the intention of creating a fully validated ODT model that can be used to generate surrogate DNS data for subsequent model reduction via PCA. Coupling the PCA model reduction technique with the ODT model (which will provide data that can serve as a statistical DNS surrogate) will provide a rigorous multiscale modeling approach.

Task 9.0 - Gasification: Char and Soot Kinetics and Mechanisms

Research will focus on three areas of emphasis: 1) expansion of the coal database, 2) characterization of char gasification rates at high temperatures in the pressurized flat-flame burner (PFFB) and 3) kinetics of the char to soot transformation of select surrogate model compounds. Reactivities obtained from a thermal gravimetric analyzer (TGA) are of interest since the chars analyzed will have been formed at high heating rates and pressures. However, the temperatures where accurate reactivities can be measured in the TGA are limited to regions with no mass transfer limitations. To date, scaling models to calculate high temperature reactivities from TGA reactivities have met with limited success. Therefore, the Recipient shall collect heterogeneous gasification reactivity data at high temperatures (>1400 K), including mass conversion rates and changes in composition, diameter and density.

The Recipient shall continue to use dimethylnaphthalene as a tar surrogate, but since it does not have all of the desired properties of an average coal tar, additional molecules will be identified that incorporate features of tar molecules (e.g. oxygen compounds, higher molecular weights). Soot yields and product gases from these model compounds will be determined. Samples produced in the PFFB will be analyzed by nuclear magnetic resonance (NMR). The Recipient will also coordinate the acquisition of high-resolution gas chromatography/mass spectroscopy (GC/MS) provided at no cost through an existing collaboration with Argonne National Laboratory. If necessary, ultra-high resolution Ion Cyclotron Resolution (ICR) mass spectroscopy data will be obtained.

Task 10.0 - Physical and Chemical Aspects of the Transformation from Char to Slag

The Recipient proposes to advance the understanding of the char-slag transformation by expanding the range of conditions and fuels from those previously studied. Based on information from previous efforts in the Utah Clean Coal Program, the Recipient shall narrow the focus on the range of conditions where the char “collapses” into slag, as evidenced by a sharp drop in internal surface area. The Recipient shall develop preliminary models to describe particle size, surface area, carbon content and reactivity near the char-slag transition point. These models will then be incorporated into the LES moment method source terms (Task 8.0).

Task 11.0 - Slag Chemistry and Slag-Wall Interactions

The objectives of this work are: 1) develop ash deposition models based on fundamental principles that are appropriate for slagging gasifiers and are sensitive to fuel properties, operating conditions, and system design, 2) outline fuel characterization techniques required to predict ash deposition behavior, and 3) continue development of computer models of coal combustors and slagging gasifiers that describe wall interactions with deposits/slags, including slag dissolution and spalling. A substantial start on the last objective comes from completed work at BYU that has been independently funded. The intention is that this work will complement the ongoing work at NETL's Albany research facility, with synergistic interactions between their experimental results and the Recipient’s modeling results. The Recipient also hopes to work with research and industrial colleagues with access to commercial or near commercial gasification facilities to compare predicted and measured results.

Activities under this task include: 1) summarizing the current state of understanding of slag-refractory interactions and critical needs to improving performance 2) developing recommendations for experimental fuel characterization, 3) generating predictive conversion techniques for the fate of inorganic material in gasifiers, 4) developing a simple model of slag-refractory interactions including chemical dissolution and spalling, and (5) comparing field and laboratory observations with predicted results of the model.

Task 12.0 - Characterization of Conditions in a 1 ton/day Entrained-Flow Gasifier for Simulation Validation

The Recipient shall acquire a first set of data from the 1 ton/day gasifier. Specifically, the Recipient shall thoroughly characterize product gas composition as a function of oxygen/fuel ratio and total pressure for one specific coal. The Recipient shall also measure the reactor wall temperature at two locations. Finally, the Recipient shall initiate efforts to sample gas composition within the reactor, using the six sampling ports along the length of the gasifier. This will allow us to characterize variations in gas composition as the fuel is converted.

Chemical Looping Combustion Reactions and Systems Thrust Area

The Chemical Looping Combustion (CLC) Team will continue previous work performed under the Utah Clean Coal Program. This work entails the collection of detailed kinetics of the CLC process using gaseous fuels and oxygen carriers suitable for chemical looping. In addition to continuing fundamental kinetic studies, the Recipient shall improve the ability to evaluate chemical looping processes by adding two additional research components: 1) experimental studies of carrier performance in a laboratory-scale batch fluidized bed reactor and 2) process modeling and economic analysis of chemical looping systems.

The Chemical Looping thrust area will include three tasks:

Task 13.0 - CLC Kinetics

The CLC Team will use TGA experiments to elucidate the chemical kinetics of the copper metal/copper oxides CLC oxygen carrier system. Initially, a single gas, either oxygen or hydrogen, will be used one at a time. Experiments with gas mixtures that simulate fuels such as syngas or methane will follow. To extract activation energies, many atmospheric pressure TGA runs from moderate temperatures (600°C) to high temperatures (950°C) at different heating rates will be required. The high-pressure capability of the TGA will permit a determination of how much the rate of the metal oxidation step is accelerated by high pressures at elevated temperatures.

Task 14.0 - Laboratory-Scale CLC Studies

The CLC Team will develop a laboratory-scale, bubbling fluidized bed reactor that can be fluidized with either heated air or superheated steam. With this design, the reactor can be switched between these two streams so as to simulate circulation of solid material between the air and fuel reactors. The system will be coupled to gas analyzers for detailed analysis of the product gas. The fluidized bed system will be useful for identifying reaction behavior under process conditions, for studying the robustness (e.g., attrition resistance) of carrier materials under flowing conditions and for identifying byproducts and impurities in the product gases. After the fluidized bed reactor is constructed, the CLC Team will test gaseous fuels (natural gas and simulated syngas). The reactor will be cycled through several oxidation and reduction cycles and oxygen carrier capacity and efficiency of fuel conversion will be evaluated as a function of the number of cycles. Initially, the reactor will be tested with well-characterized carriers so that the testing procedure can be established.

Task 15.0 - Process Modeling and Economics

Simplified process models of the chemical looping combustion process will be developed using the Aspen process modeling suite. Individual process units will be modeled using the Excel interface with Aspen. The process models will allow us to estimate how a full-scale chemical looping system will perform and will help guide the research by identifying areas where more information is needed. In addition, the Recipient shall use Aspen's built-in economics package to estimate capital and operating costs for a chemical looping system where possible. Some elements will require direct interactions with vendors.

Sequestration Thrust Area

The primary objective of the Sequestration Thrust Area is to study the impact of contaminant gases on sequestration chemistry. The Sequestration Team will build on current work performed under the Utah Clean Coal Program to study the fate of CO_2 and possible associated contaminants in the subsurface by performing experiments and by conducting computer simulations.

Task 16.0 - Carbon Sequestration

As part of current Utah Clean Coal Program efforts, experiments are being performed in a newly constructed reactor to study the basic reactivity of CO_2-brine mixtures with rocks of different mineralogy and to understand the impact of the presence of SO_2 and other contaminants. Computer simulations are being performed to assess how this reactivity may impact the morphology of faults and fractures in the subsurface (and subsequently their properties) with the goal of assessing the risk of system breaches leading to CO_2 leaks.

In this task, the Recipient shall continue to focus on reactivity of minerals in the presence of realistic gas compositions. The types of mineralogical changes during sequestration depend on rock and brine chemistry and are expected to depend on the composition of the injected gas. The Recipient shall vary the rock composition systematically to reflect realistic conditions in the field (a maximum of three variations) and perform experiments with strong and weak brine solutions. The gas compositional variations will be similar to those used thus far in the project (CO_2 with SO_2, or NH_3 and/or NO_x). All the experiments will be carried out between 50-100°C. Kinetic models will be developed to explain the observations.

The Recipient shall also look at the coupling among reaction, diffusion, and mass transfer since in natural CO_2 reservoirs, the types of reactions predicted in the laboratory are observed only to a limited extent. To accomplish this task, the kinetic models will be used in subsurface reactive transport models developed at the University to Utah to determine the range of possibilities with respect to changes in fault/fracture morphology. This information can then be used in risk/uncertainty analysis.

OIL SHALE AND SANDS PROGRAM

There is renewed interest in unconventional fuel resources as oil prices climb into hitherto unchartered territory. For the purposes of this document, unconventional oil resources are defined as extra heavy oils and bitumens associated with oil sand deposits and as producible oils from oil shale resources. These resources are of critical strategic importance because most of the world's known oil sand and oil shale deposits are in North America, and the combined potential from these resources far exceeds the world's known conventional oil reserves. The majority of the oil sand deposits in North America are in Canada, where the size of the resource is estimated to be 1.7 trillion barrels with about 200 billion barrels producible using current production methods. There are also substantial deposits in the western United States, particularly in Utah, where the resource is estimated to be 8-12 billion barrels. The most significant oil shale deposits are in the Green River Formation in Colorado, Utah, and Wyoming with an estimated resource size of 1.5-1.8 trillion barrels.

Oil sands and oil shale resources will be used primarily for producing transportation fuels. In a carbon-constrained world, transportation fuel production from these resources will require an understanding of processes that occur over a wide range of length and time scales from the structure of kerogen and how its binds to an inorganic matrix to the fluid flow resulting from in situ processing in an oil sands interval that covers hundreds of acres. The Recipient shall address these technology challenges through a research program that ranges from the atomistic level to full-scale reservoir simulation and encourages coupling and integration among the various scales (Tasks 17.0-20.0). Issues specific to carbon capture for these resources will be addressed in Task 21.0. An environmentally responsible, carbon constrained development program to produce oil from these unconventional fuels will provide a much needed boost to domestic production and will serve as a strategic resource in the global tussle for energy resources.

Task 17.0 - Kerogen/Asphaltenes Atomistic Modeling

This task will lead towards the establishment of a representative three- dimensional model of the Green River oil shale kerogen by performing three-dimensional optimizations of the proposed two dimensional structures of kerogen, calculating electron densities and frontier orbitals for these three-dimensional models, and calculating swelling properties of kerogen with different organic solvents. These computational results will be correlated with experimental data that utilizes solid and liquid state 13C NMR spectroscopy, magnetic resonance imaging, TGA data on pyrolysis kinetics, small angle x-ray scattering data on mineral matter and kerogen structure (Argonne National Laboratory), and ICR-mass spectroscopy data (National High Field Magnet Laboratory). For asphaltenes in oils sands, a combination of multidimensional liquid and low temperature solid state NMR experiments will be utilized to establish the aromatic core size, the attachments per core, and the extent of stacking of these structures. These experimental data will be used to guide and validate the structure/dynamics of the asphaltenes and will be compared with results from previous models.

Task 18.0 - Multiscale Thermal Processing (Pyrolysis) of Shale

This task will focus on the next steps in making kinetic and compositional data available for in-situ and ex-situ processing models and other applications. Apart from the bench-scale experiments on cores of different sizes and with different types of feedstock, selected high-pressure TGA experiments will be performed to understand the differences between data at low and high pressures and under different reacting atmospheres. Comprehensive characterization will be performed on the samples including, gas chromatography, mass spectrometry, NMR, HPLC, and bulk analyses (densities, viscosities, refractive index, elemental analysis, etc.). Analysis of this data will include how to use the compositional information to create mechanistic pathways for the conversion of kerogen to oil, and what pyrolysis and compositional data at different scales mean.

Task 19.0 - Pore Scale Analysis of Oil Sands/Oil Shale Pyrolysis by X-ray Micro CT and LB Simulation

The significance of transport limitations in the recovery of oil by pyrolysis of oil sand/oil shale is an important consideration in the developing technology for utilization of these fossil energy resources. Research objectives include: 1) Computer Tomography (CT) characterization of the pore network structure for selected oil sand/oil shale resources, 2) Lattice Boltzmann simulation of flow through pore network structures to predict transport properties, such as permeability, and 3) CT analysis of pore network structure during pyrolysis reactions at different temperatures.

Task 20.0 - Basin-wide Characterization of Oil Shale Resource in Utah and Examination of In-situ Production Models

This task will build on both the reservoir characterization and reservoir simulation work completed thus far. With the information on reservoir heterogeneity documented using core analysis, a key question in this task is how this heterogeneity impacts production from this resource. This question can be answered using reservoir simulation tools that utilize the resource information that is available through subgrid scale and scale-bridging models. Unfortunately, reservoir simulation of thermal processes (pyrolysis, combustion, steam injection) has not utilized recent advances in multi-scale simulation. The Recipient shall build a more effective reservoir simulation tool by exploring the application of two specific areas in CFD: managing processes occurring at vastly different temporal scales (for example, reactions versus advance of the thermal front) and incorporating processes at very small length scales (pore scale, block scale, etc.) into models operating at inter-well or reservoir scale.

Task 21.0 - Oxy-Gas Combustion for CO_2 Capture in Thermal Processing and Upgrading of Oil Shale and Oil Sand

The objective of this task is to establish a multi-scale, multi-physics, simulation-based, predictive tool aimed at quantifying predictive capability for oxy-gas burner simulations for CO_2 capture technology. The main outcome is the creation of enabling simulation technology to allow transition from air-fired furnace and heater operations to oxy-gas fired applications. To achieve this outcome with confidence requires robust validation and uncertainty quantification based on the integration of terabyte data sets from massively parallel simulations with data from key laboratory and pilot-scale experiments. The Recipient shall create an LES tool for oxy-gas combustion and the shall seek collaborators to produce experimental data useful for formal V&V/UQ methodologies. The Recipient shall collaborate with NETL in-house researchers, scientists and program offices to ensure that the efforts proposed and implemented are complementary to the large body of past and ongoing work conducted at NETL.

Task 22.0 – Effect of Oil Shale Processing on Water Compositions

The work will involve performing pyrolysis experiments of Green River oil shale under different conditions (with representative of the amounts of water) and studying the resulting water chemistry. In this project, emphasis will be on the composition of the water generated. Hydrocarbons in the water phase will be analyzed using the in-house gas chromatographic analyses. Selected analyses with gas chromatography-mass spectrometry will be performed. One or two analyses of the inorganic species in the water samples will be performed.

POLICY, ENVIRONMENT, AND ECONOMICS PROGRAM

Numerous policy, legal, environmental, and economic issues are relevant to ongoing coal, oil shale and oil sands development. These issues arise in the context of existing regulatory frameworks addressing potential impacts of fuel development on air, water, land and wildlife resources, emerging regulatory frameworks for issues such as greenhouse gas emissions and carbon sequestration, and the ongoing management of co-located resources (including competing energy resources) and scarce resources (such as water) on federal lands. Analysis of the socioeconomic and economic issues and challenges facing utilization of oil shale and oil sands is also of great importance in determining how best to direct further development of these resources. Placing scientific analysis of future coal, oil shale and oil sands development in the context of acknowledged and anticipated legal, environmental, and economic issues is critical to developing sound energy policies for the continued development and utilization of these resources. Three tasks will be conducted as part of this program area.

Task 23.0 - Climate Change Legislation and Regulatory Gap Assessment

Coal-fired power plants increasingly face opposition both through litigation and regulatory uncertainty. At the same time, it is clear that coal is certain to be a paramount resource, even in a carbon-constrained world, as the nation's population and power demands continue to expand. Thus, a critical question is the legal and socio-economic position that coal will assume as we move toward climate regulation.

This task will begin the assessment of that question by analyzing coal in the context of current and potential climate regulatory regimes. Specifically, the assessment seeks to identify restraints that such regulation may create for the continued use of coal and gaps in proposed and existing legislation that could act as impediments to such use, including the evaluation of:

- What legal and economic barriers possible federal and leading state climate regulatory regimes (e.g., carbon tax, cap and trade, direct GHG emission regulation) could create for the use of coal with and without CCS technology.

- The ways in which such legislation specifically addresses, encourages, or discourages, or fails to address, implementation of CCS technology.

- The ways in which such legislation specifically addresses, encourages, or discourages, or fails to address, implementation of "bridge" coal technologies before CCS can be implemented (e.g., promotion of more efficient and lower-emission technologies, such as IGCC, or promotion of plant construction more amenable to CCS retrofit).

- What treatment state public utilities commissions have given or refused to give thus far to cost-recovery of newly constructed coal plants, and uncertainties that such treatment creates, including with respect to current deployment of less emission-intensive coal plants and future CCS use.

- Uncertainties or other regulatory gaps that public utilities, electric merchants, and others involved in the industry perceive in reaching deployment of less emission-intensive coal plants and CCS technology, in addition to questions of liability for CCS, and potential legal and legislative solutions to such uncertainties and gaps.

This task aims to draw an initial legal and policy roadmap that may be used as extant and new coal plants move into an increasingly carbon-constrained world. Without an understanding both of how emerging legislation is likely to address coal-fired generation and of the uncertainties that industry perceives in these new regulatory regimes, industry, policymakers, and the public alike lack the necessary information to make informed judgments to allow for rational, efficient planning of the next generation of power plants. This task seeks to begin providing that assessment from the perspective of coal and CCS technology. Completion of the task should help identify specific regulatory gaps that demand more detailed and in-depth analysis going forward.

Task 24.0 – Market Assessment of Heavy Oil, Oil Sands, and Oil Shale Resources

At the request of the DOE Office of Oil and Gas per the recommendation of the Federal Advisory Committee on Unconventional Oil and Gas (Sect. 999), 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. This assessment will emphasize resources from the lower 48 states and from Alaska using the most current data available from the United States Geological Survey (USGS) and from state agencies.

The Recipient shall draw on the technical expertise accumulated by the researchers in the tasks being performed under the Policy, Environment, and Economics Program and the Oil Shale and Sands Program to:

- Develop various market penetration scenarios for existing recovery options/technologies for heavy oil, oil sands, and oil shale.

- Identify infrastructure needs that are required for future development of all three resources under various production scenarios (e.g. refining, pipeline, water and power capacity).

- Determine the impact of these various scenarios on air quality, land use, and water resource demand and quality.

- Identify and analyze the current the technology, economic, environmental, legal and policy factors limiting future development, production, and utilization of heavy oil, oil sands and oil shale.

- Investigate emerging production technologies for heavy oil, oil sands, and oil shale to determine technology readiness and provide a comparative analysis to existing recovery technologies.

- Identify opportunities to mitigate adverse environmental impacts that impede industry growth and the technical, regulatory and economic gaps that must be overcome to promote environmentally sound, safe sustained development of the nation’s unconventional resources.

- Prepare an assessment report based on an integrated, interdisciplinary analysis of these finding and distribute it to policy makers and to the public.

- Prepare and present technical papers disseminating the individual findings in each of the disciplinary areas of this project.

This assessment will complement "A Technical, Economic, and Legal Assessment of North American Heavy Oil, Oil Sands, and Oil Shale Resources," published last year by the Utah Heavy Oil Program, which provided current information on resource size, production and upgrading technologies, and the regulatory and economic climate surrounding development of these resources.

Three subtasks will also be utilized in the assessment. Additional material for the assessment will be obtained from researchers involved in Tasks 17.0-22.0.

Subtask 24.1 - CO_2 Emissions

One important selection criterion for the nation's energy supply in the future will likely include its carbon footprint, and carbon-based fuel standards are currently being discussed in several states. Both coal utilization and oil sands production generate more CO_2 per unit of energy than many competing energy sources. For example, in western Canada, greenhouse gas emissions from oil sands bitumen production (40 kg/bbl from surface mining, 65-80 kg/bbl from in-situ processes, 75-90 kg/bbl for upgrading) are much higher than from conventional oil and gas production and will soon exceed the CO_2 emissions from all other sources in Alberta. This subtask aims to collect available CO_2 emissions data from coal combustion (conventional PC, oxy-fuel and IGCC) and from the production of oils sands- and oil shale-derived liquid fuels. This work will be divided into three primary activities:

- Perform a literature review of CO_2 footprint data from energy generation by coal combustion and from production of liquid fuels from oil sands/oil shales. While much of this data is available for coal combustion technologies, this activity will track updates and will gather background data to begin estimating CO_2 emissions from an oil sands/oil shale industry in the U.S.
- Fill in the gaps in the CO_2 data. Using the data gathered during the literature review as well as process knowledge from working with the Oil Shale and Sands Program, the Recipient shall estimate CO_2 emissions from an oil sands/oil shale industry in the U.S. for the most likely extraction and processing technologies.
- Analyze 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.

Subtask 24.2 - Policy Analysis of the Canadian Oil Sands Experience

This subtask will 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. This analysis will address the impacts of the governmental differences, the differences in funding and investment mechanisms relied upon in the Canadian model as compared to those contemplated for a domestic oil sands industry, and the contrasting market realities facing the oil sands industry in Canada and in the U.S. Additionally, the task will evaluate the differences in the legal protections (and consequent management obligations) afforded the lands on which the oil sands resources are located in Canada and the U.S., as well as the regulatory frameworks for oil sands production in Canada as compared to the U.S. This analysis will also consider the practical and policy implications of domestic oil sands development continuing to proceed on state rather than federal land, as is currently the case. The subtask will 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 will 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.

This subtask will address the policy, legal, and economic considerations that are relevant to development of an oil sands industry in this country and will identify where the Canadian experience is instructive and where it is not relevant. In keeping with the overall program objectives, this task will address the practical and policy implications of elevated greenhouse gas emissions associated with oil sands production, provide legal, environmental and policy analysis of the issues associated with developing an oil sands industry in the United States, and contribute to education and information dissemination efforts.

Subtask 24.3 - Policy Analysis of Water Availability and Use Issues in the Context of Domestic Oil Shale and Sands Development

This subtask will assess the current water consumption estimates for commercial oil shale and oil sands industries and place those estimates in a legal and economic context. The focus of this effort will be on the water resources of Utah. However, due to the complex legal framework, the study will encompass the Upper Colorado River Basin where these resources reside and where future water resources are projected to be severely constrained. From a legal perspective, the subtask will 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 the water resources of the Colorado River. Additionally, the subtask will 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 and oil sands activities. From an economic perspective, this task will analyze the potential socio-economic and economic impacts and costs of water reallocation to promote commercial oil shale and oil sands activities.

Task 25.0 - Oil Sands/Oil Shale Repository of Data, Information, and Software

One of the tasks completed in a separately funded project was the release of an on-line repository for information, data, and software relating to unconventional oil resources in North America. The on-line repository, based on the DSpace software platform, has been live to the world since February 15, 2007. The repository can be located via Google and other search engines at http://ds.heavyoil.utah.edu/dspace/index.jsp. A map-based interface to the repository can be accessed at http://map.heavyoil.utah.edu/website/uhop_ims/viewer.htm. To populate the repository, the Recipient gathered files from a variety of sources, including a large number of documents from the Utah Geological Survey (UGS).

The next phase of the repository, to be completed as part of this project, includes three subtasks.

Subtask 25.1 – Addition of New Materials to the Repository

The Recipient shall emphasize the addition of reports, data, and software generated or acquired by tasks included in all three programs (Clean Coal, Oil Shale and Sands, and Policy, Environment and Economics). Examples include oil shale pyrolysis data, economic and policy analysis, experimental data from the entrained-flow gasifier and the oxy-fuel combustor, conference papers and presentations, and data from LES simulations of gasifiers and oxy-fuel systems.

Additionally, the Recipient shall continue collaboration with UGS and NETL to provide significant additional materials on unconventional fuels to the repository. The Recipient shall pursue additional collaborative efforts with other institutions to enhance the breadth and depth of repository offerings and to ensure that the repository complements the efforts of other ongoing data collection efforts such as those within the NETL Office of Research and Development.

Subtask 25.2 – Improvement of Map Server Interface to Repository

The software (ArcIMS) for the unconventional fuels map server is current but the technology is mature. We will either upgrade the map server with a soon-to-be-released version of ArcIMS or purchase new map server technology called ArcGIS Server. Both the new version of ArcIMS and ArcGIS Server are fully compatible with the GIS data in the current map server. ArcGIS Server is potentially advantageous because it is well suited for geodatabases, and several of the projects outlined in this document will provide geodatabases as one of their deliverables. However, some of the functions we have put in place through ArcIMS would require additional programming in ArcGIS Server. ArcIMS will only read specific instances of the geodatabase model, but it is possible that this limitation may be removed with the new release. Hence, we will evaluate both types of software once they have been released before making a decision on how to upgrade the map server platform.

Once the new platform is in place, we will work to increase functionality of the map server, such as adding the geodatabase models provided by Task 20.0 and Subtask 25.3. The various geodatabase models are complex. There are many levels ranging from simple single user versions to advanced enterprise instances, so implementation of these models will require careful thought. This enhanced map server will be a valuable tool to access not only the repository but also various types of data.

Subtask 25.3 – Water Solutions for Future Unconventional Fuel Development

This subtask includes several activities. In the first activity, the Recipient shall extend current work by continuing to acquire, modify, compile metadata, and create new water-related GIS datasets in cooperation with researchers in the Oil Shale and Sands Program. The Recipient shall focus specifically on the Uinta Basin in Utah and shall use existing collaborations with USGS, UGS, and other entities to ensure the accuracy and relevancy of the data. Datasets will be uploaded to http://map.heavyoil.utah.edu/website/uhop_ims/viewer.htm.

In the second activity, the Recipient shall create a geodatabase system that is compatible with ESRI® GIS software. The first step will be the development of a data needs catalogue that includes data details and metadata and an outline of additional data needs (e.g. continuous in situ observations, water quality sampling, remote sensing) necessary to support adaptive water resources management. The data needs catalogue will guide the construction of the geodatabase schema. The geodatabase will be defined to facilitate analysis and modeling activities in support of long-term water management in response to unconventional fuel industry expansion, urban growth, and energy generation. In the third activity, the Recipient shall upgrade the GIS software being used for the map server and will extend the capability of the map server with the addition of GIS datasets related to unconventional oil and to general geography.

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
- An LES tool for the combustion of coal in an oxy-fuel combustor in the near-burner region with simplified burner geometry, i.e., coaxial jets. It will include two-phase reactions and radiation as well as a full particle size distribution in the LES, which will employ the method of moments technique with the direct quadrature method of closure.
- A preliminary set of validation data for the oxy-fuel combustor, including inlet and outlet temperatures, flame length and shape, and the dependence of size-segregated ash composition on wall temperature.
- Qualitative comparison of the results from the LES tool and from the validation data
- An assessment report that identifies and analyzes barriers (economic, technology, legal, etc.) in bringing domestic heavy oil, oil sands, and oil shale resources to market.
- Reservoir models for three different in-situ processes considering reservoir heterogeneity as determined by the basin-wide characterization of the Green River formation that incorporate compositional data and kinetics determined from the kerogen pyrolysis experiments. Results will include recovery, effect of heterogeneity, and energy balance.
- An expanded repository that includes additional materials obtained from UGS, from projects funded as part of this Program, and from other sources. In addition, the map server interface will be expanded to include water resources.
- Preparation and dissemination of separate policy reports addressing three tasks/subtasks in the Policy, Environment, and Economics Program (Task 23, Subtask 24.2, Subtask 24.3). These reports may, in turn, generate one or more law review and other journal articles.

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.

The Recipient shall provide and present a technical paper(s) at the DOE/NETL Annual Contractor's Review Meeting, as necessary, held at the NETL facility located in Pittsburgh, PA or Morgantown, WV, or at an alternate location mutually agreed upon by the NETL Project Officer and the Recipient.