

STATEMENT OF PROJECT OBJECTIVES

UTAH CLEAN COAL CENTER

A. OBJECTIVES

The Utah Clean Coal Center's mission is the generation of scientific and technical information to allow for the clean and efficient utilization of coal in a carbon-constrained world. Building on the existing core-competencies developed over a long history of basic and applied research in coal science and combustion processes, the Utah Clean Coal Center (UC³) proposes to support DOE's goals in the following five thrust areas:

- Simulation – developing a new generation of large-eddy simulation (LES) based, entrained-flow computational fluid dynamic (CFD) models and developing a validation and verification environment that integrates experimental results and submodels developed in the thrust areas.
- Mercury control – providing mechanistic understanding and kinetic rates for sorbents of interest to DOE and integrating these submodels into NETL's models of sorbent injection.
- Oxy-fuel combustion – exploring effects of variations in the partial pressure of O₂ and CO₂ on coal jet ignition in retrofit oxy-coal combustion applications and providing fundamental rate parameters and sub-scale model validation for circulating fluidized beds (CFBs).
- Gasification – providing data that will address two problems encountered in entrained-flow gasifiers, those of the shorter than desired lifetimes of the refractory linings and the lower efficiencies of carbon conversion.
- Sequestration – studying the impact of contaminant gases on sequestration chemistry and vertical mixing of CO₂ and brine.

B. SCOPE OF WORK

Although remarkable progress has been made in developing technologies for the clean and efficient utilization of coal, the biggest challenge in the utilization of coal is still the protection of the environment. Specifically, electric utilities face increasingly stringent restriction on the emissions of NO_x and SO_x, new mercury emission standards, and mounting pressure for the mitigation of CO₂ emissions, an environmental challenge that is greater than any they have previously faced. The Center will address issues related to innovations for existing power plants including retrofit technologies for carbon capture and sequestration (CCS) or green field plants with CCS.

UC³ will be led by an executive committee, consisting of the Director, co-Director, and leaders from each of the five thrust areas. Industrial and technical advisory boards (including State and Federal government personnel as well as scientists and engineers from universities) will help to evaluate technological challenges and make recommendations to the Center executive committee. Each of the thrust area leaders will oversee the experimental and simulation activities and ensure their integration. The Center will partner with NETL researchers to integrate the UC³ projects with those at NETL, using simulation as the vehicle for integration and innovation. UC³ is also committed to distributing its results and to providing students trained in coal utilization technology tuned to the environmental constraints that we face in the

future. With the increased importance of coal for energy independence, training of graduate and undergraduate students in the development of new technologies is critical.

C. TASKS TO BE PERFORMED

The tasks in this section are organized into thrust areas.

SIMULATION (Tasks 1.0 through 4.0)

In this thrust area, the UC³ Team will develop a new generation of LES based, entrained-flow CFD models and a validation and verification environment that integrates experimental results and submodels developed in the other thrust areas. The UC³ Team is committed to working with NETL researchers to integrate the UC³ projects with those at NETL, using simulation as the vehicle for integration and innovation. Software developed under UC³ will be open source. The Simulation effort is organized into the following tasks and subtasks.

Task 1.0 – Identification of an Appropriate LES Algorithm and Suitable Framework for the Computations

This task involves two components: the identification of the algorithm and the deployment of the algorithm in a parallel framework. The LES algorithms are expected to effectively capture the important time and mixing scales that control many important phenomena in oxy-fuel combustion and gasification applications. Existing LES models will be evaluated to determine the proper momentum closure technique for the intended applications as defined in collaboration with NETL. Once the LES model is identified, the Simulation Team will integrate the LES model, along with other CFD components, such as the pressure projection algorithm and grid scheme, into a suitable computational framework. The framework should offer the ability to perform large parallel computations (greater than 512 processors) and offer structured adaptive mesh refinement (AMR) infrastructure.

Task 2.0 – Verification of the LES Code

Verification is the process of ensuring proper mathematical behavior of the equations in their discrete form as computed by the computer code. The Simulation Team will use the method of manufactured solutions (MMS) to define non-trivial, known exact solutions to test: 1) for programmer error and 2) that the discrete equations converge to the numerical order as defined by the associated discrete scheme for each forcing term. This task includes defining manufactured solutions that range from simple two-dimensional and three-dimensional constant density solutions to full three-dimensional solutions that vary velocity, density, and temperature. While recognizing that continuous verification must be performed while the algorithm and submodels are developed, the Simulation Team will show verification results for individual discrete time and space terms, as well as an overall order of convergence for the algorithm once the code is implemented into the framework.

Task 3.0 – Development of Stand-Alone, Multiphase ODT Submodel with Appropriate Manifold Parameters

The Simulation Team will demonstrate a stand-alone, one-dimensional turbulence (ODT) calculation that accounts for the two-way coupling of the two-phase flow consistent with the ODT model formulation. The Simulation Team will also identify the appropriate resolved-scale manifold parameters that characterize subgrid chemistry and transport and translate the physics from the subgrid scales to the resolved scales. Task 3.0 is organized into three subtasks.

Subtask 3.1 – Identification of the ODT Algorithm

The Simulation Team will identify the ODT algorithm that will best describe the subgrid physics in oxy-fuel combustion and gasification.

Subtask 3.2 – Verification and Validation of the ODT Code

The stand-alone ODT code will first be verified and validated without particles. The Simulation Team will then integrate two-phase flow into the ODT model with a simple one-way coupling. This multiphase flow model will be validated using an identified coupled problem. A two-way coupling will then be incorporated into the ODT model formulation such that a dense particle simulation will be effectively modeled. Additional validation of the two-way coupled ODT model will include a rigorous testing of the particle trajectory and particle deposition models. The goal of this testing is to effectively capture the relevant physics occurring in gasifiers and oxy-fuel combustors.

Subtask 3.3 – Identification of Manifold Parameters

The Simulation Team will parameterize the manifolds constructed from the ODT submodel simulations by a fewer number of reaction coordinates than necessary for a detailed system. The identified parameters will be transported on the resolved scale and will characterize the subgrid physics effectively. Feasibility of the manifold parameters will be studied during the overall validation process.

Task 4.0 – Construction of a Validation Hierarchy based on Intended Uses and Identification of Experimental Data Requirements

Validation is the process of ensuring that the collection of conceptual models that comprise the CFD simulation match “real-world” physical behavior. The Simulation Team will work closely with the Oxy-fuel and Gasification Teams to construct validation hierarchies for the oxy-fired combustor and gasifier to facilitate validation of the computer code. The construction of the hierarchy requires a close collaboration between NETL and UC³ to define validation data that will help quantify error in the simulation and enable certification of the code for predictive use. In this manner, simulation will be used as the vehicle for integrating any relevant work performed by NETL with the efforts of UC³. Task 4.0 is organized into two subtasks:

Subtask 4.1 – Construction of Validation Hierarchies

Validation hierarchies will be constructed for oxy-fired combustors and gasifiers. Construction of the hierarchies includes decomposition of the intended use into subsystem cases, benchmark cases, coupled problems, and unit problems. The decomposition scheme will identify and isolate key physical phenomena or coupled physical phenomena that will be used to predict simulation error of the intended use. During the process of creating the validation hierarchy, the Simulation Team will collaborate with local and NETL researchers in identification of the validation requirements, including hierarchical problem definition, as well as determining key validation data requirements that will serve as validation metrics for the various hierarchical levels.

Subtask 4.2 – Validation Hierarchy Demonstration using a Coupled Problem

Lower hierarchical level validation will be demonstrated. The demonstration calculation will be a coupled problem with the associated unit problems. This demonstration will require validation data from literature and/or existing experimental data from local and/or NETL researchers. A validation metric will be defined to measure the performance of the demonstration. Using the validation metric, a simple

sensitivity study, such as a grid convergence test, will be performed. Examples of validation demonstrations include a subgrid validation problem or a multiphase LES validation. Subgrid validation problems could include validation of the ODT subgrid model using direct numerical simulation (DNS) literature data from a geometric configuration, such as channel flow, which is similar to that found in oxy-fuel combustors and gasifiers. An LES validation problem could include a simulation of cold air and coal particles, using the two-phase LES subgrid closure, model and comparing results against the readily available literature data.

MERCURY CONTROL (Tasks 5.0 through 7.0)

In the Mercury Control thrust area, UC³ will attempt to provide mechanistic understanding and kinetic rates for sorbents of interest to DOE and will integrate submodels into NETL's models of sorbent injection.

The mercury control effort is organized into the following tasks and subtasks.

Task 5.0 – Determination of the Capacities and Rates of Adsorption of Sorbents in Packed-Bed Studies

The adsorption isotherms and rates of adsorption will be used to generate submodels for existing full-scale models of activated carbon injection. We will model physical equilibrium adsorption using, for example, the Langmuir, Freundlich, and Kible-Corrigan isotherms. Adsorption rates will be modeled with expressions patterned after the Langmuir approach:

$$\frac{d\theta}{dt} = k_{ad}C(1-\theta) - k_{de}\theta$$

where θ is the fractional coverage of adsorption sites, t is time, C is the gas-phase concentration, and k_{ad} and k_{de} are the rate constants for adsorption and desorption. For the Langmuir isotherm, equilibrium is described by

$$\theta = \frac{KC}{1+KC} \text{ and } K = \frac{k_{ad}}{k_{de}}$$

Subtask 5.1 – Review/Summary of Existing Oxidation and Adsorption Data and Models

The Mercury Team will review and summarize existing data and models for oxidation, catalytic effects, and adsorption of mercury on fly ash and carbon, including bromine impregnated carbon. The extensive fixed-bed studies of Dunham, DeWall, and Senior (2003)¹ will serve as a starting point for this work, as will the comprehensive homogeneous and heterogeneous models of Niksa and Fujiwara (2005)². This information will be used to determine if there are critical gaps in the data, especially with regard to the effects of NO_x and SO_x.

¹ G. E. Dunham, R. A. DeWall, C. L. Senior, Fixed-Bed Studies of the Interaction between Mercury and Coal Combustion Fly Ash, Fuel Processing Technology, vol. 82, no. 2, pp 197-213, 2003.

² S. Niksa, N. Fujiwara, Predicting Extents of Mercury Oxidation in Coal-Derived Flue Gases, J. Air & Waste Manage. Assoc. vol. 55, pp 930-939, 2005.

Subtask 5.2 – Evaluation of Mercury Analyzer

The Mercury Team will evaluate and modify (if needed) the University of Utah's mercury analyzer to operate in the presence of sulfur, NO, and bromine, which can interfere with the performance of the mercury analyzer's conditioning system. The University of Utah's Tekran 2537A mercury-vapor analyzer includes a wet-chemistry impinger to speciate between elemental and oxidized mercury forms. Other researchers have found that bromine interferes with traditional mercury sampling conditioning systems. This task will incorporate what they have learned to upgrade our existing conditioning system. In addition, recent testing at the University of Utah has shown that NO_x and SO_x reduce oxidized mercury species in KCl impinger solutions. While the mechanisms are analogous to those seen in wet scrubbers where the oxidized mercury is reduced in the scrubber solution, causing the emission of elemental mercury, the Mercury Team will investigate several possible solutions to this problem.

Subtask 5.3 – Fixed-Bed Experiments

The Mercury Team will perform fixed-bed experiments and analyze the data to extract rate constants for heterogeneous mercury oxidation, with and without brominated sorbents. The University of Utah's existing system, which is capable of speciated mercury measurements, will record the amount of mercury exiting the packed bed. The exit concentrations will determine the breakthrough time and the solids will be analyzed to allow for material balance comparisons and as part of Task 7.0. The effects of specific gas-phase constituents, namely chlorine, bromine, sulfur dioxide, and NO, will be studied individually and in combination. Flue gases will be generated by burning mixtures of methane, air, chlorine, and bromine. The concentrations of NO and SO₂ will be adjusted by adding them to the combustion air. The SO₂ concentrations will be representative of low, medium, and high sulfur coals. The effects of SO₃ will be examined by inserting a SCR or other catalyst bed in the reactor in the 650-800°C temperature range in future years.

Subtask 5.4 – Modeling of Full-Scale Performance

Full-scale performance will be predicted using plug-flow, heterogeneous and homogeneous reaction models, and integration with DOE NETL's ACI Field Test Program. Full-scale time, temperature, and concentration data for validation of submodels will be selected in consultation with the DOE project officer. At the present time, DOE's full-scale simulations use a Langmuir adsorption isotherm and Fluent. The Mercury Team will work with NETL to incorporate the results from Subtasks 5.1-5.3 into their simulations to improve and validate their approaches.

Task 6.0 – Identify the Effects of Gas Composition on Mercury Kinetics and Capture in Entrained-Flow Systems

In full-scale applications, sorbent is injected into the flue gas, and fixed beds are rarely employed (the packed bed, however, acts similarly to a filter cake in a baghouse). The entrained-flow experiments will allow another method of determining adsorption and oxidation kinetics, and may reveal rate-limiting intraparticle processes that are not apparent in fixed-bed experiments. These fixed-bed and entrained-flow experiments will be one of the first conducted under the same gas constituent conditions in the same laboratory. The flue gases will be generated by burning mixtures of methane, air, chlorine, and bromine. The concentrations of NO and SO₂ will be adjusted by adding them to the combustion air.

Subtask 6.1 – Evaluation of Entrained-Flow Mercury Reactor

The University of Utah's entrained-flow mercury reactor will be evaluated and modified as needed. Modifications include those for the mercury analyzer and listed in Subtask 5.2 plus additional needs to feed fly ash and carbon into the entrained-flow reactor.

Subtask 6.2 – Entrained-Flow Mercury Reactor Experiments

Experiments on the adsorption and heterogeneous oxidation of mercury in the entrained-flow mercury reactor will be performed. Some of the selected sorbents will contain bromine while some will not. The experiments will include measurements of the adsorption characteristics, namely sorbent to mercury ratios and time/temperature histories. From these experimental measures in the entrained-flow reactor and results from the fixed-bed experiments (Subtask 5.3), transport mechanisms and limitations can be determined. The experimental conditions (chlorine, bromine, sulfur dioxide, and NO concentrations) in this task will be the same as those in Subtask 5.3.

Subtask 6.3 – Integration into Heterogeneous and Homogeneous Reaction Models

The heterogeneous and homogeneous reaction models will be modified to account for any additional rate-limiting steps (i.e., due to transport phenomena) and/or catalytic surface reactions. These will then be included in the models as outlined in Subtask 5.4.

Task 7.0 - Development of Mechanistic Insight into the Chemical Bonding between Mercury and Ligands used as Model Compounds

NMR data coupled with theoretical calculations will be utilized to study the chemical bonding interactions, which will then be extended to sorbents utilized in packed-bed and entrained-flow studies. Using solid-state NMR studies of ^{199}Hg complexes and ^{13}C chemical shift tensor principal values of the ligand will enable the Mercury Team to arrive at a more detailed understanding of the nature and stability of various mercury-sorbent complexes. For example, the details of the bonding between heavy metals and ligands have recently been demonstrated at the University of Utah NMR laboratory wherein the theoretical calculations of the electronic structures demonstrate a high correlation with the ^{13}C chemical shift tensor principal values of the ligand.

Using model compounds that can serve as surrogates for the sorbents used in mercury-capture technology, it may be possible to describe more accurately the details of the molecular orbitals that are formed when mercury bonds to a sorbent/ligand. While mercury compounds are hazardous and must be handled with care, it is possible to utilize the principal values of the chemical shift tensors of both mercury and carbon to investigate the details of the bonding structure between surrogate sorbent model compounds and mercury. The results of these studies may point the way to the utilization of more efficient and stable mercury-ligand complexes.

The Mercury Team will analyze samples from Subtask 5.2 (packed-bed experiments) and correlate these with modeling results. The Mercury Team anticipates that too little solid material will be obtained from the entrained-flow reactor for NMR study. This will be re-evaluated once the entrained reactor and the NMR protocol have been established to determine if these samples can be utilized as well.

OXY-FUEL COMBUSTION (Tasks 8.0 and 9.0)

The primary focus of the Oxy-fuel Combustion Thrust Area is to investigate the effects of variations in the partial pressure of O₂ and CO₂ on coal jet ignition in *retrofit* oxy-coal combustion applications and to provide fundamental rate parameters and sub-scale model validation for circulating fluidized beds (CFBs). The experimental oxy-fuel studies will focus on the same suite of four common fuels, as described and characterized in Subtask 11.1. The oxy-fuel combustion effort is organized into the following tasks and subtasks.

Task 8.0 – Investigation of the Effects of O₂ and CO₂ Partial Pressure on Coal Jet Ignition

In this task, the effects of variations in the partial pressure of O₂ and CO₂ on coal jet ignition in *retrofit* oxy-coal combustion systems will be investigated via the following subtasks.

Subtask 8.1 – Design and Construction of an Oxy-coal Combustion Furnace

The Oxy-fuel Team will design, construct, and troubleshoot a new down-fired, 100kW, oxy-coal combustion furnace with quartz windows for optical access, which will permit flame detachment studies and future optical diagnostics. The new furnace will simulate the environment experienced by pulverized coal jet flames in boilers and will provide for the systematic control of burner momentum and velocity variables, as well as wall temperatures. It will consist of an oxy-fuel combustion chamber, followed by downstream controlled temperature cooling to simulate practical furnace conditions. The furnace will allow stabilization of axial Type 0 (no swirl) pulverized coal, diffusion flames, through the use of heated walls, and variations of oxygen content of transport and secondary air streams.

The Oxy-fuel Team will perform preliminary screening tests to confirm that the new laboratory combustor, under air combustion conditions, creates flame shapes, and NO_x emissions typical of some practical units. This is designed to support the hypothesis that this combustor creates the near burner aerodynamics typical of some practical units.

Subtask 8.2 – Coal Jet Ignition Experiments

The relationship between O₂ partial pressure in the transport stream and in the secondary oxidant stream, and the near-burner aerodynamics, flame stability and detachment, will be investigated and quantified. The experiments will focus on the effects of P_{O₂} in the transport stream, on flame stability, ignition stand-off distance, and NO_x in the exhaust. The experimental conditions will include those expected for retrofit oxy-coal combustion configurations: a normal pulverized coal particle size distribution, a representative transport fluid stream, and O₂/CO₂ mixtures for the secondary oxidant stream. The secondary oxidant stream P_{O₂} will remain constant at the “typical value”, expected for oxy-coal retrofit applications.

The Oxy-fuel Team will also study the effect of P_{O₂} within the secondary oxidant on the flame stability, ignition stand-off distance, and NO_x in the exhaust. This will involve a series of tests for each of two values of partial pressures in the transport stream, namely 1) the minimum P_{O₂} that allows a *stable* flame (regardless of stand-off distance) to be maintained, and 2) the minimum P_{O₂} that allows an *attached stable* flame to be maintained, as determined from prior experimentation. Care will be taken to minimize confounding effects of changes in velocity, momentum, and temperature, although the effects of each of these variables will also be determined.

Subtask 8.3 – Preliminary Validation of Coal Jet Ignition Models

Validation of current models of coal jet ignition as a function of P_{O_2} in both transport and secondary “air” streams will be explored using the preliminary data collected in Subtask 8.2. The Oxy-fuel Team will interpret the results from Subtask 8.2 in light of known mechanisms of coal-particle ignition and coal-particle transport in axial diffusion flames. For example, small particles gather on the outside of the jet and would therefore have their ignition mechanisms enhanced by the P_{O_2} in the secondary air stream. Careful examination of the systematically gathered data in Subtask 8.2 should allow the confounding effects of changes of temperature, velocity, and momentum to be determined.

The Team will delineate the requirements of a simulation model that both predicts the data obtained and that can be used to predict the retrofit of oxy-coal combustion to practical units. Additional experimental data required to validate such a model shall be identified.

Task 9.0 – Development of Fundamental Rate Parameters for Circulating Fluidized Beds

In this task, fundamental rate parameters and sub-scale model validation for CFBs will be provided via the following subtasks.

Subtask 9.1 – Development of a New Single-Particle, Fluidized-Bed Reactor

Fundamental rate parameters under oxy-coal fluidized bed conditions will be determined. To accomplish this, the Oxy-fuel Team will design and construct a single-particle, fluidized bed reactor (SFBR). This reactor will utilize as a basis the design of a similar reactor constructed previously at MIT by Sarofim and co-workers. The MIT group used this reactor to study fuel nitrogen conversion for coal combustion in fluidized beds. The SFBR will also provide char oxidation rate parameters as a function of temperature, P_{O_2} and P_{CO_2} for use in modeling coal in oxygen-blown CFBs. This effort is intended to support ongoing MFIX modeling efforts at DOE/NETL.

Subtask 9.2 – Collection of Experimental CFB Data for Model Validation

Pilot-scale, hot-flow CFB data will be obtained for MFIX validation. The Oxy-fuel Team will first modify the University of Utah’s existing 300 kW CFB, which has been used for various fuels in the past, but not coal. This task consists of the addition or modification of several items that will allow coal firing in preparation for subsequent efforts. These modifications include the addition of: a coal feeding system, an improved ash removal system, provisions for in-bed cooling, a heat exchanger for the flue, additional air lines (transport air, overfire air), and provisions for additional temperature and pressure measurements.

Discussion with developers of the CFB modeling tools at DOE/NETL indicated a need for hot-flow model validation data to complement the cold-flow data obtained in the NETL facility. The Oxy-fuel Team will conduct these measurements while firing natural gas only, to be consistent with current MFIX capabilities and thus provide data of near-term benefit. Anticipated measurements include: highly detailed pressure, temperature and bed voidage mapping, and semi-detailed gas composition and velocity mapping.

GASIFICATION (Tasks 10.0 through 12.0)

The overall aim of the Gasification thrust area is to improve the understanding of coal conversion in high-pressure, high-temperature, entrained-flow gasifiers, and to develop simulation submodels for such systems. These goals are achieved through several technical tasks, which will be carried out on a suite of

four coals spanning the range of properties of those likely to be used in coal gasification systems in the U.S.

Task 10.0 – Coal Conversion Studies

The objective of this task is to improve the understanding of coal conversion under high-temperature, high-pressure gasification conditions. Individual particles of coal will be pyrolyzed and gasified in well-defined laboratory-scale environments to obtain new and relevant data on coal devolatilization rates and yields, char properties, char gasification kinetics, and soot formed during pressurized coal gasification.

Subtask 10.1 – Investigation of Pressurized Pyrolysis and Char Conversion

Chars will be generated in a pressurized flat-flame burner (PFFB) at various pressures (to 15 atm), temperatures (to 1700K), and residence times (to 5 sec), and these will be analyzed for volatiles yield and physical properties. These measurements at high heating rates will enhance the existing chemical percolation devolatilization (CPD) model. These chars will also be tested for moderate temperature TGA reactivity (char-CO₂ and char-H₂O) at the same pressure as the char formation pressure.

Subtask 10.2 – Investigation of Soot Formation during Gasification

The Gasification Team will improve the understanding of soot formation from coal tar under gasification conditions using atmospheric and PFFB. Model compounds will represent coal tar, and these will include nitrogen and sulfur-containing species. The compounds will be exposed to high temperatures and heating rates in the flat-flame burner systems. The resulting soot will be captured and analyzed by GC-MS and HPLC to determine approximate compositions and molecular weight distributions. Functional group transformations, particularly of nitrogen and sulfur species, will be studied by NMR spectroscopy. Finally, the O₂, H₂O and CO₂ reactivities of the soot will be measured in a pressurized TGA.

Subtask 10.3 – Investigation of Char Burnout

In this subtask, the Gasification Team will study char burnout and development of fly ash at the end of char conversion, focusing on particle stickiness as a function of carbon content. A series of chars with varying carbon contents will be prepared by reacting chars formed in Subtask 10.1 with carbon dioxide. The Gasification Team will investigate sticking propensity as a function of carbon content, as well as morphology (scanning electron microscopy analysis) and internal surface area. Stickiness will be determined using a lab-scale drop tube reactor operating under inert conditions and having a heated probe at the outlet.

Task 11.0 – Study the Effect of Ash Characteristics and Deposition on Refractory Wear

The objectives of this task include characterizing a suite of fuels representative of potential gasifier feedstocks (four fuels) using standardized and advanced characterization techniques, development of algorithms that describe deposit and surface sintering, melting, and reactions with alkali material, and collection of literature useful for submodel validation describing deposit behaviors (heat flux, porosity, growth rate, composition, etc.) from commercial- or pilot-scale gasifiers.

Subtask 11.1 – Coal Selection and Characterization

In conjunction with other tasks and collaboration partners, a suite of four fuels suitable for this investigation will be identified. In addition to the various detailed characterizations of these fuels performed in other tasks, each of these four fuels will be submitted to proximate, ultimate, ash chemistry,

forms of sulfur, heating value, and chemical fractionation analyses. All but the last of these are standardized procedures, and the last of them is in process of standardization at ASTM. The Gasification Team will develop new fuel characterization techniques necessary to predict deposit formation and describe quantitatively inorganic material transformations in both oxidizing and reducing high-temperature environments. The results of these analyses will provide indications of chemical species compositions of the inorganic fractions of each fuel and form a database from which subsequent work will be developed.

Subtask 11.2 – Modeling of Coal Ash Sintering and Melting

Deposit sintering and melting algorithms including alkali-silica interactions appropriate for gasifiers will be developed. The algorithm will indicate the rate of sintering and its impact on strength, effective thermal conductivity, and similar deposit properties. Literature data will be used to validate the sintering and melting submodels developed, and the fuel characterization from the first subtask will be combined with existing particle models and new transformation models being developed under other sponsorship to estimate gas-phase species compositions and their impacts on materials. The Gasification Team will also develop a melting model, possibly as part of the same submodel, and based on thermochemical equilibrium descriptions of inorganic phases.

Subtask 11.3 – Acquisition of Data for Melting Model Verification

Reliable literature data from commercial- and pilot-scale gasification facilities will be obtained for melting model verification. These data are likely to be limited to deposit thickness and composition as a function of operating conditions (pressure, temperature, and fuel) and design.

Task 12.0 – Develop and Validate Computational Modeling Tools to Accurately Simulate Entrained-Flow Gasifiers

The objective of this task is to develop computational models, suitable for incorporation into computational fluid dynamic (CFD) models, which describe coal conversion and associated performance of pressurized, entrained-flow coal gasifiers. The V&V (verification and validation) approach will be used to focus the modeling efforts and to ensure that the computational models represent the behavior of a full-scale pressurized entrained-flow gasifier.

Subtask 12.1 – Heat Flux Modeling

Operational experience will be combined with data from Tasks 10.0 and 11.0 to develop submodels, suitable for integration into CFD code, for calculation of heat flux in the injector and near-wall regions. A well-recognized challenge in high temperature gasification systems is achieving good fuel conversion, which is enhanced by high temperatures, while avoiding material (i.e., refractory and injector) degradation, which is exacerbated by high temperature. In addition, slurry injection notoriously causes atomizer/injector wear in gasification systems. The objective of this subtask is to develop a model to calculate heat flux to the injector and refractory walls of the gasifier (and the injector erosion rates). The Gasification Team will identify relevant parameters responsible for heat flux, and the Gasification and Simulation Teams will develop preliminary submodels describing these and associated integration strategies. This subtask will rely on close collaboration with investigators in Tasks 10.0 and 11.0, and data generated in those tasks will be used to develop and refine the computational model.

Subtask 12.2 – Entrained-Flow Gasifier Modification

This subtask involves modifying the University of Utah's existing development-scale (1 ton/day) pressurized, entrained-flow gasifier so that it can operate on coal. Most of the modification will center on designing and constructing a coal feed system.

SEQUESTRATION (Tasks 13.0 and 14.0)

The primary objective of the Sequestration Thrust Area is to study the impact of contaminant gases on sequestration chemistry and vertical mixing of CO₂ and brine. The Sequestration effort is organized into the following tasks and subtasks.

Task 13.0 – Impact of Contaminant Gases on Sequestration Chemistry

In this task, the impact of contaminant gases on sequestration chemistry will be studied by measuring reaction rates for CO₂, brine, and rocks in a newly designed high-temperature, high pressure experimental assembly. This task is divided into the following subtasks.

Subtask 13.1 – Development of an Experimental Assembly

A high-pressure, high-temperature experimental assembly will be developed to analyze CO₂, brine and rock reactions. This high-pressure (5000 psia) and high temperature (300⁰C) reaction cell will enable the study of contaminant gases on sequestration reactions. Selective ion electrodes to track individual anions and cations will be placed in the pressure vessel, with signals collected into a data acquisition system through a pressure-seal. The types of electrodes will vary according to the type of mineral(s) used in the experiments.

Subtask 13.2 – Study of Reaction Kinetics for CO₂, Brines and Rocks

The Sequestration Team will perform experiments to study the kinetics of the reactions between CO₂, brines and rocks. Brine compositions and rock mineralogy will be chosen so that both dissolution and precipitation phenomena can be studied. Rocks of different mineralogy (calcite, dolomite, magnesite, anorthite, etc.) with well-established compositions (using x-ray diffraction) will be placed in the high-pressure cell. These samples will contact brines of known compositions and CO₂. In the first-year, one representative rock mineralogy and a single brine composition will be examined at two temperatures and one pressure. Applicability of the data at lower temperatures by extrapolation will be studied.

Subtask 13.3 – Investigation of the Effect of SO₂

The experiments described in Subtask 13.2 will be repeated with contaminant gases to identify differences in the reactions and reaction rates. The idea is to determine the dissolution/precipitation tendencies of the realistic gas mixtures in comparison to the pure CO₂ stream. Only the presence of SO₂ in the flue gas will be studied. The capability of studying other contaminant gases (H₂S, NH₃, NO) is available if there is future interest.

Task 14.0 – Study the Vertical Mixing of CO₂ and Brine

The Sequestration Team will study the vertical mixing and equilibration times using two different commercial simulators for subsurface injection and transport. Simulations have shown that due to the density difference between carbonated brine (denser and at the top) and brine (lighter and at the bottom) gravity-driven plumes of CO₂-laden water result, enhancing the mixing process in the formation. There is some uncertainty in the development and progression of these plumes, which significantly impacts the overall time of equilibration in an aquifer. The Sequestration Team will benchmark this process by studying the equilibration using two different commercial numerical simulators. We would use GEM-GHG from Computer Modeling Group and TOUGH-REACT.

Task 15.0 – Overarching UC³ Activities

The PI and co-PI will oversee UC³ activities and ensure their integration with DOE's mission. To support these overarching activities, UC³ has organized three subtasks.

Subtask 15.1 – Form a Technical and Industrial Advisory Board

The board will comprise stakeholders to determine goals for UC³ and experts in the fields of simulation, mercury control, oxy-fuel combustion, gasification, and sequestration to evaluate the quality and productivity of the different tasks. The boards will include representatives from industry, academia, and government.

Subtask 15.2 – Host a Conference to Disseminate Results and Publish a Conference Summary

UC³ will host a conference to disseminate their work and solicit input from experts in the field. The UC³ team will summarize the highlights of the conference.

Subtask 15.3 – Prepare progress and final reports of activities

As required by DOE, UC³ will submit regular reports including: progress reports, quarterly milestone updates, and annual accomplishments.

D. CRITICAL PATH PROJECT MILESTONES (MILESTONE PLAN/STATUS)

As a part of the approved SOPO, the Recipient will develop a Milestone Plan that will be used as a planning tool to establish the time schedule for accomplishing the planned work. The Milestone Plan will serve as the baseline for tracking performance of the project and will identify critical path project milestones (no less than 2 per calendar year) for the entire project. The critical path project milestones are:

Critical Path Milestone	Planned Completion Date
Selection and standard characterization of the coals (Subtask 11.1)	2 months after award
Construction of the validation hierarchies for oxy-fuel combustion and gasification (Subtask 4.1)	3 months after award

During project performance, the Recipient will report the Milestone Status as part of the required quarterly Progress Report as prescribed under Attachment 4, Reporting Requirements Checklist, Section

4.A.7-Progress Report. The Milestone Status will present actual performance in comparison with Milestone Plan, and include:

- (1) the **actual** status and progress of the project,
- (2) specific progress made toward achieving the project's critical path milestones, and,
- (3) any proposed changes in the projects schedule required to complete critical path milestones.

E. 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:

- (1) Validation hierarchies for the oxy-fired combustor and gasifier to facilitate model validation.
- (2) The LES code and ODT submodels.
- (3) A topical report on Tasks 5 through 7 (mercury control), including mercury absorption rates for several sorbents of interest.
- (4) A topical report on Task 8 (oxy-fuel combustion) including: data on the effects of PO_2 and PCO_2 on coal jet ignition in turbulent axial diffusion flames, and interpretation of these data in the light of currently available models.
- (5) Pilot-scale, hot-flow CFB data for use in MFIIX validation.
- (6) A topical report on Tasks 10 through 12 (gasification), including: data on char sticking propensity as a function of carbon content and temperature, TGA kinetics, soot analysis, and fuel characterization.
- (7) A computer sintering algorithm with validation data describing sintering rates of condensed-phase deposits as a function of temperature and deposit composition (Task 11.2).
- (8) A topical report on Tasks 13 and 14 including: the reactivity of CO_2 -brine-rock systems with and without the presence of SO_2 ; and how vertical mixing is modeled in different subsurface reactive transport codes and how this representation can be improved.
- (9) A summary of the conference discussed in Task 15.2.

F. BRIEFINGS/TECHNICAL PRESENTATIONS

The Recipient shall prepare detailed briefings for presentation to the DOE Project Officer at NETL facilities in either Pittsburgh, PA or Morgantown, WV. Briefings shall be given by the Recipient to explain the plans, progress, and results of the technical effort. At a minimum, the Recipient shall prepare a detailed briefing for presentation to the DOE Project Officer at NETL facilities in either Pittsburgh, PA or Morgantown, WV for the project kick-off meeting and for the final project review briefing.