National Energy Technology Laboratory

Office of Research and Development

Capabilities and Facilities Related to Gaseous Multi-Component Capture

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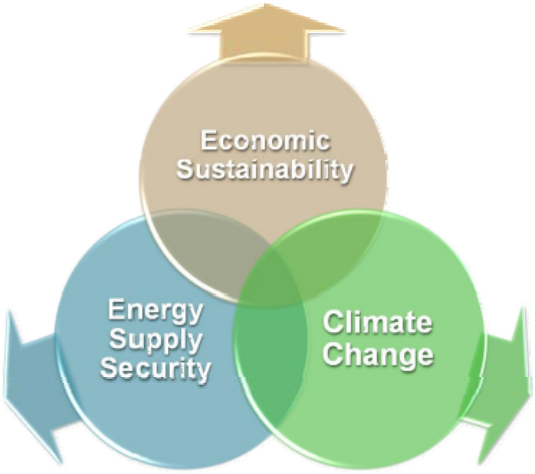

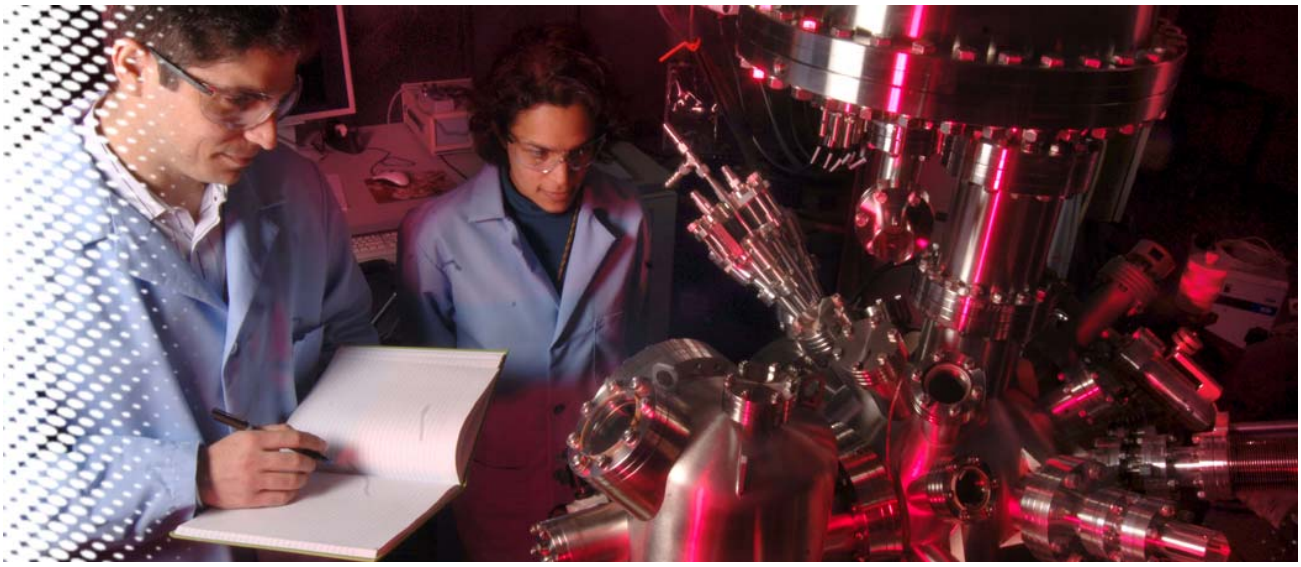

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1. Overview of NETL and ORD

1.1. Introduction

The National Energy Technology Laboratory (NETL), part of DOE's national laboratory system, is owned and operated by the U.S. Department of Energy (DOE). NETL supports DOE's mission to advance the national, economic, and energy security of the United States. Specifically:

> NETL research enables domestic coal, natural gas, and oil to economically power our Nation's homes, industries, businesses, and transportation, while helping to protect our environment and enhance our energy independence.

To fulfill its mission, NETL implements a broad spectrum of energy and environmental research and development (R&D) programs that will return benefits for generations to come. NETL has expertise in coal, natural gas, and oil technologies, contract and project management, analysis of energy systems, and international energy issues. NETL's impact is demonstrated by the fact that nearly 75 percent of the Nation's coal-burning power plants incorporate NETL-derived technologies.

NETL's research portfolio includes projects conducted on-site by its Office of Research and Development (ORD) as well as R&D conducted through partnerships, cooperative research and development agreements (CRADAs), financial assistance, and contractual arrangements with universities and the private sector. Together, these efforts focus a wealth of scientific and engineering talent and a unique research infrastructure on creating commercially viable solutions to national energy and environmental problems.

In addition to scientific research, NETL offers a energy analysis capability. NETL's Office of Systems, Analysis and Planning (OSAP) conducts continuing energy analyses that provide input to decision makers on issues such as national plans and programs, resource use, environmental and energy security policies, technology options for research and development programs, and paths to deployment of energy technology.

1.2. Role of ORD at NETL

ORD supports DOE's Office of Fossil Energy (FE), other DOE Offices, other federal agencies and private entities with on-site research at advanced facilities in Morgantown, WV, Pittsburgh, PA and Albany, OR.

Over the years, ORD has achieved recognition for:

- Providing solutions to key national energy challenges – CO_2 management, advanced fuels development, hydrogen technology, hybrid cycles, mercury capture, hydrates
- Capitalizing on unique facilities and capabilities
- Achieving breakthrough science – Computational science and application, hydrogen technologies, combustion science and engineering, sequestration mechanisms
- Achieving technology successes – R&D 100 awards, technology transfer awards, publications, licenses, etc.

ORD provides an on-site "corporate laboratory" that utilizes state-of-the-art capabilities and facilities. ORD employs a core group of about 200 Federal scientists and engineers, supplemented by contractors who are selected through a competitive process, as well as research fellows and associates at the faculty, postdoctoral, graduate, and undergraduate levels.

ORD provides:

- A flexible, focused research effort that addresses national fossil energy R&D needs
- Impartial evaluation of new concepts and materials and expert authoritative review of external R&D proposals
- A venue for universities, other Federal agencies, and other research organizations to participate in collaborative research
- In-depth expertise in technologies and research methodologies for program planning and management purposes
- Hands-on fossil energy technology training for experienced postdoctoral researchers, graduate students, visiting professors, and undergraduate students
- A wide-ranging set of collaborations with regional and national universities on fossil energy research issues

Currently, ORD's on-site research efforts are making significant contributions in addressing key energy and environmental issues, including secure and reliable energy, future roles for hydrogen, clean power generation from coal, global climate change, and critical infrastructure assurance.

1.3. Doing Business with ORD

ORD welcomes opportunities to work with the private sector, public sector, and academia to develop and commercialize energy and environmental technologies. ORD has a great deal of experience promoting the use of federally-funded knowledge, facilities, and capabilities.

ORD can structure a wide range of relationships with the private sector to further develop and commercialize technology that originates in the laboratory for the benefit of the nation. For example, ORD frequently uses CRADAs to do cooperative work with industry. Each partner in the CRADA applies the agreed-upon resources, such as personnel, equipment, and/or facilities. CRADAs are mutually beneficial because: ORD and the participant can negotiate intellectual property (IP) disposition, such as rights to patents, protection of information, and exclusive or non-exclusive licensing of inventions.

In addition to CRADAs, ORD can enter into license agreements for applying ORD inventions. The ORD can also use its laboratories and scientists in work-for/with-others arrangements. For example, ORD is partnering with universities on other DOE missions and other federal agencies including the National Aeronautics and Space Agency (NASA), the Department of Defense (DOD), and the National Science Foundation (NSF).

ORD also regularly works with industry groups and other partners to sponsor technical conferences, meetings, and workshops. Also, ORD maintains an online library of technical publications and software tools, and conducts on-going education and technology transfer activities in keeping with its role as a government owned and operated national laboratory.

The following examples highlight some of the partners and collaborators with whom ORD has relationships:

- Research and Development Solutions, LLC. (RDS) – Consortium of EG&G, Parsons, and SAIC that provides ORD research support.
- CWP, Inc. – University consortium (Carnegie Mellon University, West Virginia University, University of Pittsburgh) partnering with ORD through RDS.
- Pittsburgh Technology Council – Membership of 1,400 across southwestern PA, makes it one of the largest regional trade associations of its kind in the nation.
- Innovation Works – State-sponsored regional development organization whose mission is to increase the new-enterprise success rate in southwestern PA.
- PA Nanomaterials Commercialization Center – Initiates/establishes/promotes R&D of nanomaterials S&T; ORD serves on Technical Advisory Committee.
- TechConnectWV– WV nonprofit that facilitates commercialization of IP from laboratories and universities.
- DOE Regional Carbon Sequestration Partnerships – Partnerships formed under DOE sponsorship to test advanced carbon control and sequestration technologies in a variety of geological settings, ORD scientists and engineers are collaborating with several partnerships.
- Solid-State Energy Conversion Alliance (SECA) – National organization that promotes and develops advanced fuel cell technologies under DOE sponsorship ORD researchers are working with the SECA members.
- Power System Development Facility (PSDF) – Research facility supported by NETL to test advanced gasification and related energy technologies. ORD conducts key simulation studies in support of PSDF.

1.4. ORD Organization

ORD is a matrix organization in which research leaders plan and manage R&D projects that are carried out by research staff that report administratively to line managers. The creation of synergism through shared responsibility between project and functional management allows ORD to respond to new challenges in a positive and proactive manner. The ORD Director provides overall direction and leadership to ORD research leaders and managers. These leaders and managers, in turn, plan, manage and implement R&D in support of DOE's energy and environmental missions; develop and maintain technical R&D core competencies; design, construct, operate, and maintain the Laboratory's R&D facilities; oversee site support service contractors; coordinate activities of research associates and visiting scientists; actively seek external partners for activities involving on-site facilities or research staff; and develop cooperative research opportunities.

Within ORD, research project ideas are conceived and work plans are developed within Focus Areas. Focus areas are designed to provide a nationally-recognized scientific authority and leadership in each specific thrust area. A Focus Area is a collection of research activities and capabilities, focused on a particular set of energy issues, applications or research thrusts that is matrixed across the organization allowing ORD to share key personnel and unique research facilities in multiple areas. Focus Areas are dynamic and can be refocused in response to significant shifts in energy research. Each Focus Area has a Focus Area Leader (FAL) who is responsible for the planning, development, funding and technical leadership, including annual

planning, long-term planning, portfolio development, capability development, and technical quality assurance.

Currently, there are four ORD Focus Areas and two smaller research areas. These areas are:

- Focus Areas
    - Computational and Basic Sciences
    - Energy System Dynamics
    - Materials Science
    - Geological and Environmental Systems
- Other research areas
    - Gas Hydrates
    - Ultra Deep/Unconventional Gas and Oil

ORD's line management is organized into ten Divisions that share staff and resources to address Focus Areas. The Divisions represent core competencies and key scientific and engineering disciplines, and are managed by Division Directors who are experienced in the appropriate competencies as well as in management of personnel and resources. The ORD Divisions are:

- Earth and Mineral Sciences
- Separations and Fuels Processing
- Energy System Dynamics
- Engineering Research
- Environmental Science
- Geosciences
- Chemistry and Surface Science
- Computational Science
- Materials Performance
- Process Development

1.5. ORD Capabilities and Staffing

ORD conducts world-class R&D in a variety of areas in the energy and environmental sectors. ORD's capabilities are exemplified first and foremost by a cadre of highly educated and experienced scientists and engineers with skills in experimental and computational science, supported by expertise in design and operation of facilities ranging from laboratory research to bench-scale advanced design and testing. While the remainder of this document emphasizes the ORD facilities, the actual capabilities go far beyond the hardware. The highly trained, dedicated research staff, together with the up-to-date research facilities described below present a formidable capability to develop solutions to the Nations energy challenges.

ORD is led by a core staff of federal researchers, with the following disciplines strongly represented by Ph.D. level research scientists and engineers, many with national reputations in their fields:

- Chemical Engineering
- Chemistry
- Physics
- Mechanical and Aerospace Engineering

- Geology and Geosciences
- Mathematics
- Materials Science and Engineering

ORD is a participant in the Institute for Advanced Energy Research (IAES), a contractual relationship formed through Research and Development Solutions, LLC, with Carnegie Mellon University, the University of Pittsburgh and West Virginia University. The NETL-IAES has evolved into an ORD-based research organization with approximately 25 faculty members and 100 Ph.D. students and postdocs, and funding of approximately $12 million per year. An additional 50 faculty members and their students collaborate with ORD-IAES faculty or directly with ORD research scientists based at the ORD laboratory sites. All university personnel involved in its research programs have a direct affiliation to the ORD through the IAES. The expertise and excellence of the research staff has been recognized by conferring the title of Fellow of the organization upon many of them.

1.6. Research Focus Areas – Summary Level Descriptions

Computational and Basic Sciences (CBS)

CBS activities integrate physical and chemical experimental research with computational sciences to understand and develop technologies, advanced materials, and multi-scale energy systems ranging from the molecular-scale to device-scale to plant-scale. Focus area activities include assembling computational models from ab initio (atomic and molecular) through device-scale, and to integrate the device-scale models into virtual plant simulations. The CBS focus area supports activities in coal power systems, natural gas and oil technologies, and also strives to meet national energy security goals.

Energy System Dynamics (ESD)

ESD activities conceive, analyze, and develop pre-commercial energy technology to minimize the environmental impact of fossil fuel use and maximize domestic energy sources and infrastructure. The focus area primarily addresses in plant devices, such as fuel cells, turbines and fuel cell hybrids, fuel processors for fuel cells, gasification, carbon dioxide capture technologies for pulverized coal, technologies for integrated gasification combined cycle (IGCC) systems, reciprocating engines, and advanced sensor/control methods. The ESD focus area conducts research and development in coal power systems in support of the President's Global Climate Change Initiative.

Materials Science

This focus area addresses the need for new or improved materials that can withstand higher temperatures, pressures and corrosive environments of new power generation technologies such as coal gasifiers, advanced turbines, combustors, and fuel cells. Materials Science activities involve life cycle research, starting with the design, formulation, melting, and characterization of metals, alloys, and ceramics; casting and fabrication; prototype development; and the recycling and remediation of waste streams associated with these processes.

Geological and Environmental Systems (GES)

GES activities involve geological sequestration of carbon dioxide; resources assessment; production modeling; development of unconventional gas and oil resources; fate of air toxics

such as mercury; by-product utilization; and water issues related to oil and natural gas extraction and existing coal-fueled electric power plants. GES focus area efforts also involve collaborative activities with the regional sequestration partnerships developed by DOE. GES performs research in carbon sequestration technologies, natural gas and oil technologies, and clean power generation in support of the President's Global Climate Change Initiative.

Gas Hydrates Research Area

Methane hydrate is a crystalline combination of natural gases and water. Scientists estimate that the energy locked up in methane hydrate deposits is more than twice the global resources of all conventional gas, oil, and coal deposits combined. ORD has experience and capabilities in determining the physical properties of natural gas hydrate samples collected either in the field or produced in the laboratory, and ability to incorporate this data into improved geologic and numerical models of gas hydrate behaviour in natural settings. ORDs work supports the DOE's effort to understand the role hydrates play in global processes such as climate and the carbon cycle; the impact of hydrates on seafloor stability and deep-sea life; tools and knowledge that will ensure the safety of drilling and producing deep-water oil and gas resources located below marine hydrate deposits; and the knowledge and technology base to allow commercial production of methane from domestic gas hydrate deposits.

Ultra Deep/Unconventional Gas and Oil Research Area

In the Ultra Deep and Unconventional Gas and Oil area, ORD has developed unique capabilities to study drilling under extreme conditions; evaluate the environmental impacts of oil and natural gas development; develop processes for enhanced and unconventional oil recovery; and conduct resource assessment. The research activities have been formulated in association with the research and development effort established by Title 9, Subtitle J, of the Energy Policy Act of 2005. The goal of the work is to identify and remove technological barriers to expanded domestic oil and gas resource utilization. The activities also focus on developing quality educational opportunities for student training. To ensure that research efforts are not duplicated, ORD personnel work closely with the external Research Partnership to Secure Energy for America (RPSEA) consortium.

1.7. Summary of ORD Capabilities

Table 1, beginning on the following page, provides a road map to the detailed descriptions of ORD capabilities in the sections that follow.

Table 1 - Summary Table of ORD Capabilities

Focus Area	Capability Area	Capabilities/Facilities/Models
Computational and Basic Science (CBS)		
	Computational Chemistry	Ab Initio Molecular Orbital Calculations First Principles Density Functional Theory Calculations Classical and Quantum Molecular Dynamics Simulations Grand Canonical Monte Carlo Simulations Kinetic Monte Carlo Simulations
	Computational Fluid Dynamics	Device Scale Modeling Computational Multiphase Flow MFIX, open-source software C_3M – Carbonaceous Chemistry for Continuum Modeling Gas-solids Flow Experiments for Model Validation
	Process and Dynamic System Modeling	Advanced Process Engineering Co-Simulation (APECS) Dynamic Simulation and Control
	High-performance computing and visualization	Computational Software Computing clusters Visualization facilities
Energy System Dynamics (ESD)		
	Separations Technology	Sorbent and Membrane Development Novel Capture Processes for CO_2 and Contaminants Bench-scale Sorbent Testing
Materials Science (MS)		
	Materials Characterization	Analytical Facility with SEM, TEM, XRD, WDXRF, XPS or ESCA, DTA, FTIR, ICP, AA, HPLC, etc.
	Surface Science	Advanced Surface Analysis and Imaging System Spectroscopy Laboratories Physisorption and Chemisorption Structural Analysis - X-ray Diffraction Laser Nano Particle Lab
	Reaction Chemistry and Engineering	Hydrogen Separation and Production Nano and Materials Synthesis Materials Physical Properties and Small-scale Processing Fuels and Catalysts
Geological and Environmental Sciences (GES)		
	Environmental Research	Coal By-Products Leaching Lab Trace Metals Lab Ambient Air Quality Monitoring

2. ORD Capabilities by Focus Area

2.1. Computational and Basic Sciences Capabilities

Scientists in the CBS focus area have extensive experience in quantum mechanical simulations, atomistic/molecular dynamics, advanced materials and fuels research and development, mesoscale simulation, multiphase flow simulations (MFIX code), device-scale simulations using computational fluid dynamics (CFD), advanced process engineering co-simulation (APECS), integrated virtual plant modeling, and model validation testing at each scale.

2.1.1 Computational Chemistry

Development of efficient future technologies for energy production with zero carbon emissions based on the use of fossil fuels or novel renewable resources is highly dependent on solving a large number of individual breakthrough tasks in diverse number of areas. These range from identification of new materials for gas capture, storage or separation to optimization of energy use and transformation processes. ORD's Computational Chemistry Group has the capabilities to provide atomistic insight into behavior of materials and chemical processes and correlate the atomic and molecular scale structure and property information to practical performances of materials and processing conditions of interest for various technologies developed at NETL. The capability addresses a diverse number of systems and chemical processes ranging from catalysts development for fuels from coal (hydrogen and others), development of dense membrane systems with improved gas transport properties, surface corrosion, and fuel cell processes, to novel nanostructured materials for gas storage and separation (e.g., hydrogen separation, CO_2 separation and absorption).

These capabilities include a variety of quantum and classical computational methods. Among the portfolio of computational chemistry capabilities used by the group are Ab Initio Molecular Orbital Calculations, First Principles Density Functional Theory Calculations, Classical and Quantum Molecular Dynamics Simulations, Grand Canonical Monte Carlo Simulations, and Kinetic Monte Carlo Simulations. Based on these methods the group is able to provide unique atomistic information about the structural properties of bulk systems and their surfaces, stability and performance properties of bimetallic alloys, description of chemisorption properties in both homogeneous and heterogeneous processes or prediction of dynamical and transport properties in either gas, liquid or solid phases.

ORD has developed state of the art computational and visualization facilities fully dedicated to the research activities performed by Computational Chemistry Group. These include a diverse number of Intel and AMD-based Beowulf cluster systems with modern communication capabilities like InfiniBand and Myrinet. Additionally, the members of the group perform research at Pittsburgh Supercomputing Center as members of SC2 (Supercomputing Science Consortium) and on a variety of supercomputing systems at various Major Shared Resource Centers within Department of Defense.

ORD's state of the art capabilities in computational chemistry integrate high performance hardware, scientific software, and advanced visualization programs, such as:

- **System Hardware:**
  - Several Beowulf clusters with a total of about 500 cores with high-speed, low-latency interconnects.
- **Scientific Software:**
  - Ab initio molecular orbital calculations: Gaussian 03, Q-Chem, Molpro
  - Periodic DFT calculations: VASP, CASTEP, DMOL
  - Molecular dynamics simulations: Discover, DL_POLY
  - Finite-element based simulations: Comsol Multiphysics.
- **Visualization:**
  - Accelrys - Materials Studio, Gauss View,
  - VMD (Visual molecular dynamics)

2.1.2 Computational Fluid Dynamics

Device Scale Modeling

This research facility uses state-of-the-art, high-speed computing resources to verify computational fluid dynamics (CFD) models used to study coal gasifiers, gas turbine combustors, solid oxide fuel cell (SOFC) systems, and liquefied natural gas plumes, as well as mercury capture technologies. DSM research is helping to move advanced visualization and high-performance computing models from researchers' computer screens to actual laboratory experiments and pilot testing.

Computational Multiphase Flow

In the laboratory, ORD researchers are using advanced computational and experimental research to develop novel technologies based on (multiphase) gas-solids flow such as transport gasifiers, circulating fluidized-bed combustors, and hot gas desulfurization. ORD has an ongoing research capability to develop physics-based multiphase flow simulations. The multiphase flow simulations provide detailed information on the flow patterns, species, and temperature distribution and help reduce the uncertainty in scale up, thereby reducing the time and cost for developing advanced gasifiers. As part of the research, vast amounts of data are rendered into a readily understandable visual form. This allows scientists to visualize the inner workings of fluidized beds, and allows engineers to make changes in the reactor design and “see” the impact of these changes on the performance of the reactor.

MFIX Open-source Software

MFIX is the result of the research work done at ORD over the last fifteen years. MFIX has been used to develop and validate multiphase flow theory (transport equations and constitutive relations) and to develop numerical techniques for solving these equations efficiently and accurately. Since making the code available to researchers, the use of MFIX has gone beyond its originally intended application, primarily gas-solids fossil fuel reactors, to other applications, such as the simulation of industrial (e.g., polyethylene reactor) and natural processes (e.g., volcanic flows).

Carbonaceous Chemistry for Continuum Modeling (C_3M)

ORD has developed a detailed Carbonaceous Chemistry for Continuum Modeling (C_3M) module that can be used with CFD models such as MFIX to describe the chemical reactions occurring in multi-phase flows that have high levels of solids loadings. C_3M was developed specifically for

use with the continuum approach. C_3M won a 2008 Federal Laboratory Consortium (FLC) National Excellence in Technology Transfer Award for its use in the analysis and design of pilot- and commercial-scale gasifiers. A patent application has been filed, and ORD is making the module available for licensing.

The C_3M module adapted for hydrogasification is called Continuum Chemistry Module for Hydrogasification (CCMH). Arizona Public Service (APS) is using the CCMH with both MFIX and FLUENT® Eulerian-Eulerian models to support design and operation of a bench scale reactor and provide modeling support for scale-up. The APS reactor will operate at very high pressures and temperatures under dilute operating conditions. The CCMH will provide APS with species concentrations under a range of operating conditions and reactor configurations. In a second application of CCMH to hydrogasification, the ORD and CE-CERT (College of Engineering-Center for Environmental Research and Technology) UC-Riverside have a CRADA to examine how the coal-steam ratio affects the syngas composition and energy requirements as well as the issue of scale-up of a hydrogasification reactor. Researchers are also interested in how the preparation of the coal affects both hydrodynamic behavior of the bed and conversion.

Gas-Solids Flow Experiments

A circulating fluidized bed (CFB) facility is used for generating data necessary for validating CFD models such as MFIX. The CFB lab is also used for physically simulating existing plants, optimize plant operation, and evaluate innovative designs and operations. Researchers study solids mixing, and transfer and control issues that are commonly encountered in most advanced power generation systems.

The cold-flow CFB is capable of simulating a fully integrated system for solids transfer and control. The cold-flow unit consists of a riser, a two-stage cyclone, standpipe, and a 2 ft diameter fluidized bed (FB) with an associated cyclone and make-up hopper. Transport lines connect these vessels in a variety of configurations with mechanical and non-mechanical solids control valves. The main riser is 1 ft diameter, 56 ft high, and consists of metal and acrylic spool pieces. ORD's cold flow facility is equipped with advanced instrumentation that measures detailed flow structures and regimes, solid/gas velocities and concentrations at various points within the reactor. ORD's current solids-flow device uses a rotating spiral for measuring solids circulation rate.

The facility has a supply of 250,000 scf/h air with the ability to obtain superficial velocities of 10 to 30 ft/s in the riser, and 0.2 to 0.7 ft/s in the FB. The operating pressures range from 0 to 15 psig at the riser outlet and up to 30 psig in the FB. The FB vessel is pressurized so that a representative differential pressure can be attained between the FB and the riser.

The device is also used for developing novel measurement techniques. Currently under development is a device for High Speed Particle Image Velocimetry. ORD scientists have developed a high speed particle imaging technique for visualizing dense gas-particle flows, solids velocity, solids concentration, and granular temperature.

2.1.3 Process and Dynamic System Modeling

Process & Dynamic Systems Research focuses on predicting the steady and dynamic behavior of advanced energy processes at the scale of the power plant.

APECS with ANSYS Engineering Knowledge Manager

APECS (Advanced Process Engineering Co-Simulator) is first-of-a-kind software that helps improve performance of advanced fossil fuel power plants. APECS provides the accuracy and detail needed to understand and optimize fluid flow (e.g., from combusted coal), heat and mass transfer, and chemical reactions that drive overall plant performance. The APECS system combines steady-state simulation of fluid processes with high-fidelity equipment models. This combination effectively ensures optimal power plant performance by matching physical properties and reaction rates in both types of models.

APECS is used today by engineers and researchers in the process and energy industries, as well as academia, national laboratories, and other research entities. In the chemical industry, process engineers are using APECS to analyze the impact of complex reactor mixing and fluid flow phenomena on overall plant product quality and yield. In the power industry, cycle engineers are employing the APECS technology to develop competitive power plant solutions with significantly reduced development costs and technical risk. In the research community, scientists use APECS to develop optimization-based reduced-order models based on CFD results, to link process/CFD co-simulation to immersive 3D virtual engineering software, to perform stochastic analysis and to add multi-objective optimization capabilities for process/CFD co-simulations. APECS was developed by ORD computational scientists and engineers in collaboration with R&D technology partners, and won 2004 and 2008 R&D 100 Awards.

IGCC Dynamic Simulator Research and Training Center

The ORD is leading a collaborative R&D project to develop a full-scope, high-fidelity, real-time dynamic simulator for a generic IGCC plant with carbon capture. The IGCC simulator will combine a process/gasification simulator and a power/combined-cycle simulator together in a single dynamic simulation framework. ORD is using the simulator to establish a flagship IGCC Dynamic Simulator Research & Training (DSR&T) Center. ORD and its Collaboratory R&D partners will use the IGCC simulator to showcase clean coal technology, and to offer IGCC plant operation and control demonstrations, technology familiarization, and hands-on computer-based training.

2.1.4 High Performance Computing and Visualization

High-performance computing infrastructure and partnerships with regional science consortiums allow ORD scientists to determine a wide range of physical and chemical properties – from nanoscale molecular studies to the feasibility of commercial-scale power plants. High-performance computing at NETL is facilitated through a regional supercomputing science consortium – SC2 – between ORD, the Pittsburgh Supercomputing Center (PSC), and sponsors from academia and government, including Carnegie Mellon University and the National Science Foundation. A high-speed optical network has been established between ORD and the PSC. Researchers are able to transfer gigabytes of data from simulations completed at PSC back to ORD for post-processing and visualization in a matter of minutes. Also, ORD researchers use computational resources provided by Department of Defense and DOE's Office of Science.

ORD has a dedicated team to assist scientists in their visualization needs. Support can range from writing custom reader modules for visualization applications to helping users operate one of the display systems in the lab. The visualization capabilities at ORD include a 12-panel tiled LCD display, a large 3D immersive display, and a portable 3D immersive display. The primary scientific visualization software applications used are ParaView and Ensight. 3D Studio is used for creating 3D geometry. Chromium is used to distribute the graphics across the multi-screen displays. VTK and OpenSceneGraph are used when creating specialized visualization software. Custom in-house software is written when a data format needs to be modified or to simplify the visualization process.

2.2. Energy System Dynamics Capabilities

The ESD focus area is investigating and developing new energy system concepts and technologies, such as: technologies that can capture carbon dioxide during energy generation with minimal cost and efficiency impact, methods to use hydrogen combustion in turbines and engines without collateral pollutant emissions or efficiency penalties, performance testing of fuel cells, methods to make fuel cells tolerant to coal gas impurities, allowing fuel cell integration with coal gasification technology, SOFC fuel cell degradation related to design and operation issues, sensors and control techniques that will allow load following in hybrid turbine fuel cell systems, fuel reforming and gas cleanup technology that can allow SOFC fuel cells to operate on existing infrastructure fuels (diesel fuel, coal syngas).

These capabilities include:

- Capabilities of analyzing fuel cells to validate and establish a common approach to reporting fuel cell performance; developing methods to make fuel cells tolerant to coal gas impurities, enabling fuel cell integration with coal gasification technology; and understanding SOFC fuel cell degradation related to design and operation issues.
- Developing fuel reforming and gas cleanup technology to allow SOFC fuel cells to operate on existing infrastructure fuels (diesel fuel, coal syngas).
- Advancing technologies to capture carbon dioxide during energy generation with minimal cost and efficiency impact.
- Identifying methods for using hydrogen combustion in turbines and engines without collateral pollutant emissions or efficiency penalties.
- Developing sensors and control techniques that will allow load following in hybrid turbine fuel cell systems.

ORD researchers have applied their experience to design next-generation thermal power plants using oxy-fuel combustion and Integrated Pollutant Removal (IPR™) systems. In addition, ORD researchers have used its expertise in pollutant capture and carbon dioxide sequestration to evaluate potential carbon management strategies.

2.2.1 Separations Technology

ORD conducts a wide range of separation science and fuels processing technology research in the areas of carbon management and capture, hydrocarbon production and conversion, pollutant removal and related areas.

2.2.1.1 Sorbent and Catalyst Development

Sorbent and Catalyst Preparation Facilities

ORD has the ability to prepare sorbents/catalysts suitable for fixed, moving and fluid bed reactor applications. Equipment includes mixer pelletizer, rotary vacuum evaporator, lab scale spray dryer, dome extruder, as well as attrition testers and particle size measurement equipment.

2.2.1.2 Novel Capture Processes for CO2 and Contaminants

ORD and its university partners have the capability to conceive and develop new concepts for CO_2 capture including novel membranes, sorbents and reactor concepts for flue gas and syngas applications. These concepts include: sorbent-enhanced reaction processes, chemical looping, metal complexes, promoters, surface immobilization, and membranes.

2.2.1.3 Bench- Scale Sorbent Testing

ORD has three unique gas/solids reactors that have the capability of testing in either the fixed- or fluidized-bed configurations, and at high temperatures and low-to-high pressures. These reactors are being used to evaluate how well regenerable sorbents/catalysts remove CO_2, NO_x, mercury, and other trace elements from combustible coal gas streams.

Over the past decade, these facilities have been leaders in addressing R&D issues associated with commercialization of suitable catalysts/sorbents for gas desulfurization. ORD researchers and industrial partners use the test facility to study gas/solids reaction systems that are vital to cutting edge technologies, including CO_2 storage and energy-efficient fossil fuel utilization. It operates in conjunction with facilities for sorbent/catalyst bench-scale testing and for in-situ (in-place) reaction studies. In 2000, NETL received an R&D 100 Award for its RSV-1 Regenerable Desulfurization Sorbent. The process for preparation of this sorbent has been patented and licensed to industry.

High-Pressure Bench-Scale Fixed- /Fluidized-Bed Reactor

The reactor shell is constructed from Incoloy 800HT alloy. Inside the shell is a removable, Alonized stainless steel cage designed for easy loading and unloading of catalyst/sorbent. (Alonizing is a process for treating stainless or carbon steel surfaces with vaporous aluminum to improve corrosion resistance at high temperatures.) Three different sized cages are available, providing a unique flexibility to generate scale-up information. The online sampling instrumentation available in these facilities includes gas chromatography and mass spectrometry. Online sampling of exit gases and condensate can be done by an operator and sent to the onsite analytical lab for analysis.

Low-Pressure Bench-Scale Fixed- /Fluidized-Bed Reactor

This reactor is constructed from quartz tubing located inside a vertically positioned tube furnace. Tubing and fittings, from the mass flow controllers to the reactor, are titanium; while the tubing from the reactor to online instrumentation is titanium or Teflon. These materials render this reactor inert to most trace contaminant species. Online sampling instrumentation includes gas chromatography and mass spectrometry. Online sampling of exit gases and condensate can be taken by an operator and sent to the on-site analytical lab for analysis.

Low-Pressure Lab-Scale Fixed-Bed Screening Unit
This unit consists of an Alonized stainless steel reactor located inside a three-zoned, vertically positioned tube furnace. The small size of this reactor makes it ideal for economical screening studies, where a large number of cycles may be required or where many samples may be necessary to screen in a short period of time. Online sampling instrumentation includes gas chromatography and mass spectrometry. Online sampling of exit gases and condensate can be performed by an operator and sent to the on-site analytical lab for analysis.

2.3. Materials Science Capabilities

2.3.1 Materials Characterization and Analytical Facilities

Using ORD's capabilities in materials evaluation, researchers can characterize almost all incoming materials and outgoing products. They can determine a material's chemical and structural makeup; mechanical properties; physical properties such as thermal characteristics, particle size, porosity and permeability; surface structure; microstructure; and, corrosion, fracture, and wear characteristics. The following descriptions highlight specific areas:

2.3.1.1 The Analytical Facility

- Scanning Electron Microscopy (SEM), with Wavelength and Energy Dispersive Spectroscopy, Electron Backscattered Diffraction, and Cathodoluminescence,
- Transmission Electron Microscopy (TEM), with Energy Dispersive Spectroscopy,
- X-ray diffraction (XRD),
- Wavelength Dispersive X-ray fluorescence (WDXRF),
- X-ray photoelectron spectroscopy for chemical analysis (XPS or ESCA),
- Fourier Transform Infrared Spectrometer (FTIR),
- a full wet chemistry lab for quantitative elemental analyses of both liquids and solids,
- sequential inductively coupled plasma spectrometry (ICP),
- atomic absorption spectrophotometer (AA),
- optical emission spectrometry,
- UV/Visible scanning spectrophotometer,
- gas chromatography,
- combustion analyzers for C, H, N, S, O,
- ion chromatography for occurring anions, cations, and organic acids, and
- a high-performance liquid chromatograph (HPLC),
- Internationally recognized, award winning optical metallography laboratory for microstructure characterization and phase determination, and
- Thermo-analysis laboratory that offers dilatometry for thermal expansion measurement, Laser Flash for thermal diffusivity measurements, and DTA/DSC for measurement of phase transitions and thermodynamic properties.

2.3.2 Reaction Chemistry and Engineering

2.3.2.1 Hydrogen Separation and Production

ORD's Hydrogen Separation Facilities support research in four main areas:

1. Membrane Materials – investigate and develop materials and fabrication techniques for producing suitable membranes for separating hydrogen.
2. Membrane Performance Testing – characterize the performance of promising novel membranes by using continuous gas feed streams and conditions similar to industrial processes.
3. Water-Gas Shift Membrane Reactor Development – develop a membrane reactor for enhancing hydrogen production from the water-gas shift (WGS) reaction at high temperature and pressure with no added catalyst.
4. Advanced Separation Science – explore new concepts and conduct fundamental studies to reduce hydrogen production costs, for example, by studying CO_2 -selective membranes and the chemistry of hydrogen transport and sulfur poisoning.

State-of-the-art facilities and instrumentation include:

- Hydrogen Membrane Test (HMT) Units
- Membrane Screening Systems:
- Materials Lab
- ASPEX PSEM
- PANalytical XRD

Hydrogen Membrane Test (HMT) Units:
These units provide the unique capability of high-pressure, high-temperature hydrogen membrane flux measurements at conditions of up to 1000 psi at 900°C. The units can accommodate membrane sizes up to one inch in diameter and up to six inches in length in both disk and tubular configurations, with process gas flow rates up to 20 L/min. In addition, the HMT units have the flexibility to be used for both membrane separation testing and membrane reactor testing.

- HMT-1: dedicated to studies that utilize sulfur-laden, “dirty” gas streams without concerns about cross-contamination with clean gases.
- HMT-2: used as a “clean” system for testing with gas mixtures containing no sulfur compounds.
- HMT-3: optimized for testing membrane reactor systems.

Membrane Screening Systems
Laboratory Membrane Screening Systems (MSS) are used for small-scale, low-pressure analysis of membrane permeation under different environments, or for conditioning materials prior to subsequent characterization. For example, it allows for short-term testing of membrane materials with different sulfur-containing gas mixtures at varying temperatures.

Materials Lab
Membrane fabrication capabilities include a well-equipped laboratory for inorganic materials preparation. Equipment available for alloy fabrication includes high temperature, controlled atmosphere furnaces, precision TIG welder, arc welder, hydraulic presses, high temperature-corrosion resistant TGA, and cold plasma sputter coaters. Machine shop facilities are also available.

ASPEX PSEM
An Aspex PSEM 2000 scanning electron microscope equipped with an energy dispersive x-ray detector (EDS) is used for membrane and materials characterization. Changes in membrane morphology, element migration, layer thickness, and pore size are among the characteristics studied.

PANalytical XRD
A PANalytical X-Ray Diffraction instrument with a hot stage, cold stage, and high-speed detector is used for determining and observing membrane material crystal structure under realistic membrane conditions.

2.3.2.2 Nano and Materials Synthesis Laboratory

The Materials and Catalyst Research Laboratory's work ranges from synthesizing and characterizing novel catalysts and adsorbents to investigating their properties. The scope of materials under investigation is also wide. Scientists calculate critical parameters such as surface area, low temperature, high resolution isotherms, and isosteric heats of adsorption using advanced instruments. They can also identify Isotherms over a wide range of pressure (0–80 atm) and temperature. Spectroscopic methods are used to provide more detailed information about the adsorption sites. A specially designed and constructed variable-temperature, variable-pressure view cell is also used to obtain critical information on the specific sites responsible for adsorption.

2.3.2.3 Materials Physical Properties and Small Scale Processing Facilities

Micromeritics Autochem 2950
This fully automated chemisorption analyzer is available for temperature programmed, pulse chemisorption, and physisorption analyses of dispersed metal catalyst materials. Scientists can use it to prepare and analyze catalytic samples at pressures up to 70 bar (1000 psia). It also has a sub-ambient temperature controlled ramping capability using cryogenic cooler. It utilizes a 200 amu Pfeiffer Vacuum Thermostar mass spectrometer linked through a dedicated port to detect and identify low concentrations of condensable and/or reactive gases.

Centorr Vacuum Industries vacuum arc melter
The arc melter is used to prepare lab scale samples of alloys and other high melting point materials. The instrument utilizes an electric arc to melt and/or react high melting point starting materials under vacuum or inert atmospheres. Virtually any metal or alloy can be melted into a small ingot for further sample processing.

High-pressure reactor system (Model *MAPGLM3*)
This instrument is an automatic, computerized fixed-bed reactor system that can be operated up to 700°C and 100 bar. It utilizes an HPLC liquid pump, has automatic liquid/gas separator with level control for operation with liquids and gases at high pressure in continuous mode and an Agilent GC equipped with TCD/FID detectors, and methanizer.

Durston rolling mill
A manually operated rolling mill produces foils of softer metal alloys. It is primarily used to produce metal membrane foils.

Weld Logic Microwelder
The microwelder is designed very small or thin metals including those of nonstandard composition. It supports metal membrane development but has many other applications.

UHV Deposition Chamber 1
This UHV chamber is equipped with plasma, evaporation, and magnetron deposition sources as well as Auger Electron Spectroscopy for characterizing deposited films.

UHV Deposition Chamber 2
This UHV chamber is equipped with Knudsen diffusion cell and XPS for fabrication and characterization of thin films.

UHV Deposition Chamber 3
This UHV chamber is equipped for sample preparation, reaction and characterization.

Other materials testing instrumentation:

- Thermolyne 46200 High temperature box furnace 1700°C Material synthesis, conditioning, atmosphere: air
- Thermolyne 79300 Tube Furnace Annealing/conditioning tube furnace #1 1500°C, 3" tube, atmosphere: Inerts, 1% H2 in Ar
- Thermolyne 54500 Tube Furnace Annealing/conditioning tube furnace #2 1200°C, 3" tube, atmosphere: Inerts, 1% H2 in Ar
- Annealing/conditioning tube furnace #3 1000°C, 1" tube
- Standard muffle furnace large 1200°C
- Standard muffle furnace small 1000°C
- Optical microscopes (3)
- Denton sputter coaters (2)

2.3.2.4 Fuels Processing

Fuels processing capabilities include the ability to develop and assess liquid fuels reforming as well as gasification of solid fuels such as coal and biomass. Reforming hydrocarbon fuels is a very attractive source of hydrogen for distributed fuel cell power generation. However, this approach historically utilizes solid catalysts, which are susceptible to coke formation and sulfur poisoning from sulfur compounds present in the hydrocarbon feed. ORD's fuel processing facilities are exploring fundamental and applied reforming research and development phenomena inherent in catalytic and electro-catalytic unit operations present in fuel cell power plants. These issues include: reaction kinetics, development of fundamental reforming activity and selectivity scales, mapping reforming catalyst coking regimes, improving sulfur tolerance and understanding their mechanism of poisoning, and catalyst development and characterization.

Fuels Reforming and Processing
The fuel reforming facilities are comprised of four bench-scale reactor systems, Catalyst Screening Unit (CSU) and Fuel Processing Unit (FPU) reforming test rigs, one Micrometrics catalyst characterization unit, and state-of-the-art analytical capabilities (further details are given below). These facilities were designed as fuel flexible; natural gas, methanol, Fischer-Tropsch

fuels, diesel fuel, automotive gasoline and their surrogates may be utilized as feedstock. Catalytic materials tested in this laboratory are developed at NETL or may be provided by external collaborators.

Bench-Scale Reactor Systems

- Four identical high temperature and high pressure fixed-bed reactor systems
- Capability to run in different reforming modes such as autothermal reforming, partial oxidation, steam reforming and hydrodesulfurization of hydrocarbon compounds, and the temperature programmed oxidation and reduction of catalyst samples
- Reactor outlet streams are analyzed for the permanent gases as well as C1-C7 hydrocarbons using an online mass spectrometer and online gas chromatograph, respectively
- Two of the reactor systems are designed for 24/7 unattended operation

Reforming Test Rigs

- Capability to run in different reforming modes such as autothermal reforming, partial oxidation, steam reforming and hydrodesulfurization of hydrocarbon compounds, and the temperature programmed oxidation and reduction of catalyst samples
- Reactor outlet streams are analyzed for the permanent gases as well as C1-C7 hydrocarbons using an online mass spectrometer and online gas chromatograph, respectively
- The CSU is a multipurpose and versatile research facility and can easily be modified for evaluating the advanced concepts for fuel reforming such as plasma-assisted reforming, temperature profiling of the catalyst bed during exothermic or endothermic reactions
- The FPU has been designed and constructed for the purpose of testing 5-25 kW fuel processors developed by NETL sponsored developers, such as those in the SECA program. The FPU may also be used during collaborations with other industrial developers through CRADAs
- The FPU is also designed for 24/7 unattended operation

Catalyst Characterization Unit

- This unit performs N2 BET surface area analyses, temperature programmed reduction, temperature programmed oxidation, temperature programmed desorption, surface titrations, and chemisorption experiments
- Effluent gas can be analyzed using an online mass spectrometer

Coal/Biomass Gasification

Coal/Biomass Feed Preparation and Torrefaction

Co-feed coal/biomass gasification systems take advantage of mixtures of abundant coal and less abundant biomass (a 'CO_2 neutral' fuel) to reduce net CO_2 emissions. To effectively utilize biomass as a fuel, technology must be developed to prepare and feed biomass with a minimum amount of energy expenditure and processing steps. In addition, the physico-chemical property differences that exist between coal and biomass result in additional complexities associated with effective mixture gasification. Due to its fibrous and compressible nature, biomass is difficult to prepare for introduction into a gasifier. Torrefaction, which consists of subjecting the feedstock

to gas at temperatures of 200° - 300°C for a definite time, dries, embrittles, and renders the biomass more dense, enabling pulverization and injection.

Biomass Feed Preparation Laboratory (BFPL)
Scheduled to become operational in April 2009, it will provide the capability to torrefy and grind biomass feedstocks suitable for gasification alone or for co-gasification with coal. The torrefied biomass will be characterized by proximate and ultimate analyses, mechanical properties, and the energy expenditure required for production. These quantitative measures are essential to the rational design of co-gasification systems.

2.3.3 Surface Science

2.3.3.1 Advanced Surface Analysis and Imaging System (SAIS)

The Lab's state-of-the-art SAIS integrates a broad suite of surface analysis and imaging tools into one single vacuum chamber. Techniques supported in this single instrument include:

- X-ray Photoelectron Spectroscopy
- Ion Scattering Spectroscopy
- Low Energy Electron Diffraction
- Auger Electron Spectroscopy
- Scanning Tunneling Microscopy
- Atomic Force Microscopy

2.3.3.2 Scanning Electron Microscopy (SEM)

The laboratory has extensive SEM capabilities, including:

- FEI Quanta 600 High Resolution Scanning Electron Microscope
- Aspex LLC PSEM 2000 variable pressure scanning electron microscope equipped with energy dispersive x-ray analyzer

2.3.3.3 Spectroscopy Laboratories

Polarization Modulation Infrared Reflection Absorption Spectroscopy (PM-IRRA)
The Fourier Transform PM-IRRAS system is used to study the surface chemistry of metal foils. The system is coupled to a vacuum reaction cell capable of temperatures up to 1500 Kelvin.

Raman Spectroscopy and Microscopy
Dispersive and Fourier Transform Raman spectrometers are used to study vibrational and electronic properties. Raman spectroscopy is well-suited for high-pressure experiments and several variable-temperature, high-pressure (up to 300 atmospheres) cells are available. The Raman systems are used for in-situ studies of gas adsorption in nanoporous separation membranes. They are used extensively for studying the dissociation and formation properties of methane hydrates.

Variable Temperature and Pressure Infrared Spectroscopy
This unique, cryogenic vacuum system is coupled to a Fourier Transform Infrared Spectrometer. The vacuum chamber can sample temperatures from 5-700 Kelvin and pressures from 10^{-9} to 760 Torr. This system is used to study gas adsorption in carbon nanotubes, metal-organic frameworks, and other novel porous materials.

2.3.3.4 Physisorption and Chemisorption Instrumentation

The Lab's high-pressure isotherm capabilities include a volumetric isotherm instrument with capabilities up to approximately 150 atmospheres, as well as a gravimetric system capable of pressures up to approximately 48 atmospheres. Low-pressure instrumentation is capable of collecting high-resolution isotherms up to 1 atmosphere. Chemisorption, surface area, and pore size studies are also possible with the low-pressure instrumentation.

2.3.3.5 Structural Analysis - X-ray Diffraction

Lab scientists use X-ray diffraction to study crystalline phase identification and quantification, crystallite size determination, and preferred orientation measurements. Instrument capabilities include flexible sample stages to accommodate a range of samples and a hot stage capable of heating samples in-situ to 1200°C under vacuum or controlled atmosphere. The International Centre for Diffraction Data (ICDD) inorganic phase data base is available for routine phase identification.

PANalytical X'Pert Pro MPD powder diffractometer: The Lab's X-ray diffraction system is used to study crystalline phase identification and quantification, crystallite size determination, and preferred orientation measurements. Instrument capabilities include flexible sample stages to accommodate a range of samples and cold and hot stages capable of cooling or heating samples in-situ over the range of -193 to 1200°C under vacuum or controlled atmosphere.

2.3.3.6 Laser Nanoparticle Laboratory

ORD's Laser Nanoparticle Lab investigates complete "Green" synthesis and stabilization metal nanoparticles and nanomaterials, "Green" nanomaterials for deep oil drilling and recovery, "Green" nanofluids as coolants for power plants and energy devices
"Green" metal nanoparticles as solid lubricants and metal nanoparticles for medical applications.

The facility contains the following systems, equipment, and capabilities:

- Laser ablation to generate nano-particle materials
- Transient hot wire thermal conductivity measurements (KD2)
- Viscometer (Brookfield Engineering)
- Yield stress measurement (Brookfield Engineering)
- Dynamics Light Scattering particle size analyzer (HORIBA LB550)
- Surface tension and contact angle measurement (DROPIMAGE 250, Rame-Hart)
- Fluorescence Spectrometer (OCEAN OPTICS)
- UV-VIS Spectrometer (OCEAN OPTICS)
- Differential Scanning Calorimeter (DSC) for nanoparticle meting and surface energy measurements (Q200A; TA Instruments, Inc.)
- Pin-on-Disc Tribometer (Micro Photonics) for friction measurements

2.4. Geological and Environmental Systems Capabilities

2.4.1 Environmental Research Facilities

2.4.1.1 Coal By-Products Leaching Laboratory

Leaching Lab Capabilities:

- Batch leaching, roller technique: standard method
- Batch leaching, sequential at multi pH values: ORD developed method
- Batch leaching, parallel at multi pH values: most recent EPA-sponsored method
- Semi batch leaching columns: single batch of solid, continuous liquid feed for simulation of in-situ mono-fill
- Semi batch continuous stirred tank extraction: single batch of solid in a stirred tank with continuous liquid feed for basic chemistry/engineering studies

Analysis Instrumentation:

- Inductively Coupled Plasma – Optical Emission Spectroscopy (ICP-OES): multi element detection and quantification
- Inductively Coupled Plasma – Mass Spectroscopy (ICP-MS): multi element detection and quantification
- High Pressure Liquid Chromatography – ICPMS (HPLC-ICPMS): metal speciation
- Cold Vapor Atomic Fluorescence (CVAF): mercury specific
- Microwave Digestion: sample preparation of solids for above spectroscopies
- Thermal Gravimetric Analysis (TGA): automated moisture and ash analysis
- Automatic Titration: determination of alkalinity, capable of most common titrametric techniques including pH-stat titrations

2.4.1.2 Trace Metal Capture

(Applies to flue and fuel gas, Mercury, Arsenic, Selenium, Phosphorus)

Packed-bed reactors:

- Lab-scale reactor – outer diameter ¼-inch-by-20-inch quartz tube with flow rates from 60–120 ml/min
- Bench-scale reactor – outer diameter 1-inch-by-20-inch quartz tube with flow rates from 2–10 l/min
- Gases containing mercury include simulated flue gases, simulated fuel gases
- Mercury continuous emissions monitors (CEMs) measure mercury in the gas phase
- Cold vapor atomic absorption spectrophotometer analyzes spent sorbent
- Operating temperature: ambient to 750°F
- Photochemical Oxidation using UV light (PCO^{TM}) to capture, oxidize, and enhance removal of elemental mercury from flue gas
- Thief Process (Activated Carbon Injection)

2.4.1.3 Ambient Air Quality Monitoring and Modeling

Plume, local area and regional source – receptor and air quality modeling

- Array of stationary site and field deployed Gas species and Particulate Matter monitors available for site characterization.