Collaboratory for Multiphase Flow Research — CMFR

Program Objective:

The objective of the collaboratory is to accelerate the development of multiphase simulation capability and promote its use to enhance the success of NETL's R&D investments. This will be done by developing multiphase models and software and by conducting validation experiments as identified by an analysis of the barrier issues encountered in technologies central to NETL's mission. The collaboratory will be organized by NETL and the three local universities (West Virginia University, University of Pittsburgh and Carnegie Mellon University). It will increase collaboration with other universities and external entities and leverage funding from external agencies. The net result of this program will be a suite of validated models, expanded experimental capabilities, a methodology for combining experimental data and models to analyze problem areas, and the wide-spread usage of this methodology in the design of NETL sponsored technologies. A corollary benefit is that the collaboratory will become a world-class resource center for research in multiphase flow simulation, a much sought after capability for the power, chemical, mineral, and petroleum industries.

Justification:

Understanding and simulating multiphase flows involving solids is of critical national importance. Solids flows occur in many energy conversion processes central to NETL's mission: gasification processes, coal combustion systems, carbon capture, FutureGen power and hydrogen production, and chemical looping combustion, for example. An estimated 40%, or $61 billion, value added by the U.S. chemical industry is related to particle technology [1]. As discussed below solids-based processes are fraught with scale-up and operational problems [1, 2]. Multiphase flow simulation offers a novel way to analyze and solve such problems.

Performance problems encountered in solids processing industry are well documented. A Rand study showed a distressing drop in plant performance when solids processing steps are involved. The average design capacity of solids processing plants is 64% compared to 90-95% for gas/liquid processing plants; start-up of such plants is delayed by approximately two years [2].

Many NETL and advanced fossil energy technologies use complex solids based reactors, whose design call for much improvement in efficiency, reliability, and pollutant reduction. Solids constitute a major feedstock in NETL technologies; e.g., coal, petroleum coke, biomass, black liquor, oil shale. Solids also appear as sorbents in hot gas clean-up systems or as catalysts in shift converters. Most NETL technologies, from the existing ones to those being considered for the future, involve one or more solids processing steps; e.g., coal gasification and combustion, shale oil program, chemical looping, oxy-combustion, oxygen-free gasification, direct reduction of iron ore. Three of the four barrier issues identified by NETL are related to solids based systems. For example, reliability is the single most important technical limitation to be overcome in order to achieve widespread deployment of gasification technology [3] and problems with solids-based systems are prevalent in gasification technology. Gasifier feed injectors are considered to be the weakest links in the technology [3]. Start-up problems at the Piñon Pine project are attributable to fines handling and undesirable temperature ramp up in the gasifier [4]. Scale up of solids handling reactors is notoriously difficult [5], which, for example, manifested at Tampa Electric project as lower than expected carbon conversion [4].

Most of the solids-based processes include a carrier gas or liquid and involve chemical reactions; e.g. the burning of coal particles in a stream of air. Understanding and accurately modeling such flows would lead to greatly improved designs of multiphase flow reactors. Multiphase computational fluid dynamic (CFD) modeling has been recognized as a tool that has much potential [5]. There are numerous examples of successful application of single phase CFD models, which are routinely used in aerospace and automobile industries and increasingly being used by the chemical industry. For example, a chemical and engineered materials company concluded that, over a six-year period, the benefits accrued from the use of CFD resulted in a six-fold return on the total investment (including salaries) required in CFD [6]. But multiphase CFD is not yet well enough developed to be used by itself for scale up [5]. Therefore, it is no wonder that the Chemical-Industry-of-Future Technology Roadmap for CFD, written by representatives from the industry, identifies modeling dilute to dense multiphase flows as one of the highest priority items [7].

The above summary shows that advancing multiphase flow computational science is an area in which NETL has *technical needs*, that is of *great national importance*, and where NETL has a *proven track record* (Appendix A). The availability of tremendous intellectual capital at the *local universities* (West Virginia University, University of Pittsburgh and Carnegie Mellon University) motivates the formation of CMFR to satisfy NETL's technical needs. The vision of the collaboratory is consistent with Program Strategic Performance Goal ER 4-7 "Sustain U.S. preeminence in fossil fuel technology by supporting development of material, computational-method, and control-system knowledge needed to bridge gaps between science and advanced engineering …" and NETL's Computational Basic Science Focus Area vision to "fundamentally alter the process by which advanced energy plant concepts are developed" [8].

Approach:

There are three dimensions to the approach that will be adopted by CMFR to support NETL's mission. The first pertains to research planning. With the current level of resources and funding the NETL research groups have been able to do impressive work in developing the engineering science underpinnings (computational and experimental) necessary to support NETL technologies. However, the current level of funding has not allowed a comprehensive analysis of barrier issues particular to NETL technologies utilizing these engineering science underpinnings. The CMFR will change that by identifying specific needs and targeting modeling and experiments to develop technology-specific solutions. This will produce two beneficial effects: 1. the technology-specific solutions with a scientific basis (as opposed to a correlation of data) will be provided to an immediate problem; 2. such solutions will provide a feedback to expand the engineering science knowledgebase, which has wider applications than to the immediate problem and, in time, would have greater impact on NETL technologies (Figure 1).

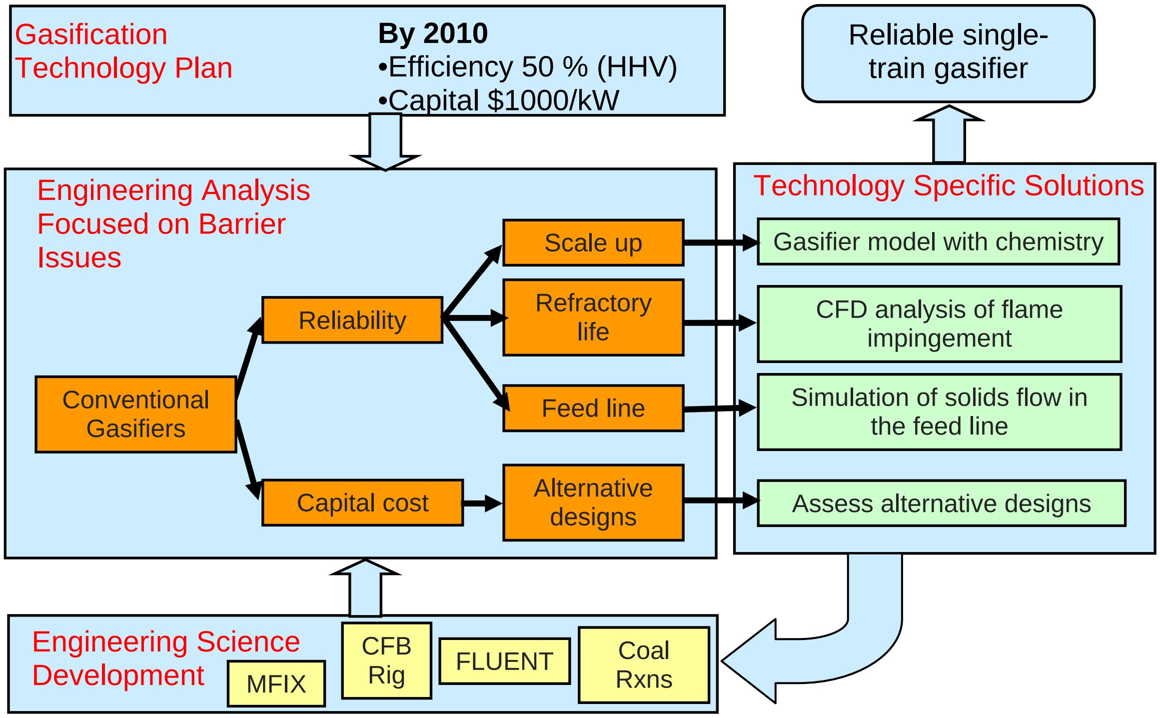


Figure 1. An example of combining a barrier issue analysis and engineering science to develop technology specific solutions. This enhances the success of that specific technology, but also expands scientific knowledge, which has much wider applications.

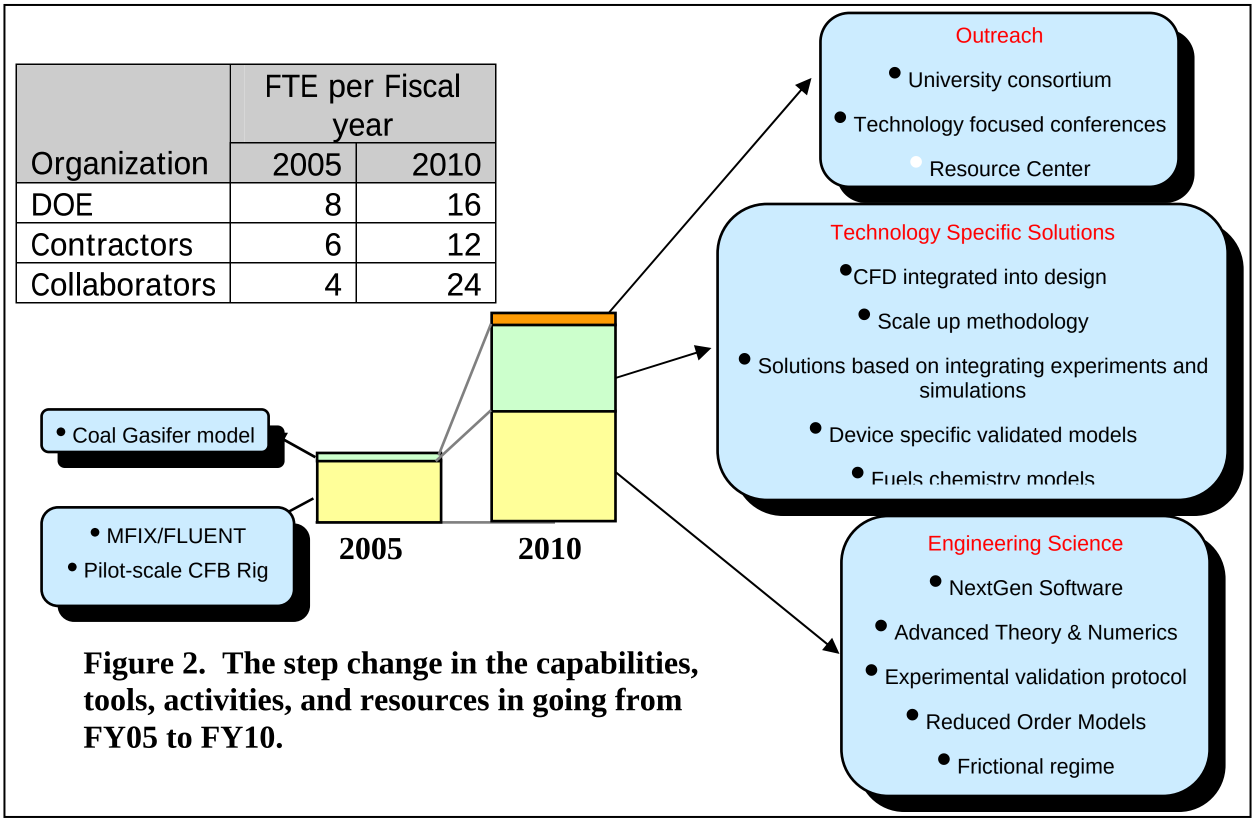
Another dimension of the CMFR approach will be a better integration of experimental and computational sciences. There are two broad sources of experimental data: one is the controlled (lab-scale) experiments such as conducted at NETL (Appendix A) and the other is pilot or demonstration scale units. The development of controlled experiments and models will be coordinated and be dictated by technology-specific needs. This activity will result in validated models for specific applications. These models may not be fully validated and may require additional information (data gaps) before they can be used to describe industrial scale units. Such gaps will be filled by using data from pilot and demonstration plants. The filling of the gaps will proceed by improving the models as well as using phenomenology. Phenomenology will serve an immediate need; the advancement of the models will expand the engineering science knowledge-base. In time less and less phenomenology will need to be used as the knowledge-base expands.

A third dimension of CMFR will be increasing the participation of external collaborators. The collaboratory will organize collaborative research, internships, and conferences. External collaborators can become a part of CMFR and contribute to the collaboratory's common goal. The collaborators will benefit by having access to CMFR resources (personnel, information, software, experimental facility, and funding) and by being able to identify technical problems suitable for external grant applications. For example, external collaborators are using NETL software to model volcanic flows, and a proposal to model the lunar and Martian regolith for NASA is under consideration. They will provide NETL an expanded pool of technical experts, the ability to leverage funding from other agencies, and the opportunity to develop future engineers and scientists to sustain the development of NETL technologies. The external collaborators will also act as peer reviewers to assure the technical quality of the work performed and as members of an advisory committee to help with the planning of research projects. The collaboratory will also conduct targeted training workshops to promote the use of computational technology so as to fundamentally alter how the design of future power plants would be done.

The above approach will result in a step change in the capabilities, tools, activities and resources in the area of multiphase flow research. Figure 2 shows the current status and the status expected by FY10. NETL's role will be to organize the research around technology specific interest areas. Research staff from NETL, support contractors and external collaborators will work on the projects. See Appendix B for an outline of tentative plans of CMFR. Detailed plans will be developed as one of the first projects of CMFR.

A summary of the benefits derived by NETL follows:

- Sustain NETL's preeminence in this R&D area
- Fundamentally alter how future power plants would be designed by promoting the use of computational technology
- Thereby, minimize the risk and enhance the success of NETL technologies
- Train and attract next generation of scientists and engineers



Organization	FTE per Fiscal year	
	2005	2010
DOE	8	16
Contractors	6	12
Collaborators	4	24

- Coal Gasifer model

- MFIX/FLUENT
- Pilot-scale CFB Rig

Outreach

- University consortium
- Technology focused conferences
- Resource Center

Technology Specific Solutions

- CFD integrated into design
- Scale up methodology
- Solutions based on integrating experiments and simulations
- Device specific validated models
- Fuels chemistry models

Engineering Science

- NextGen Software
- Advanced Theory & Numerics
- Experimental validation protocol
- Reduced Order Models
- Frictional regime

Figure 2. The step change in the capabilities, tools, activities, and resources in going from FY05 to FY10.

Budget Requirements:

The budget requirements are shown in Figure 3. It shows a growth in NETL supplied funding and an increase in the external funding starting with FY07.

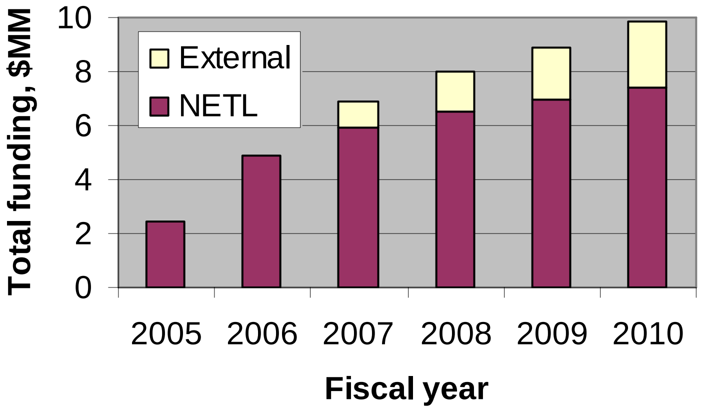


Figure 3. Funding profile for five years including expected funding from external agencies.

Strategic Partners:

The collaboratory will be organized by NETL and the three local universities (West Virginia University, University of Pittsburgh and Carnegie Mellon University) and will eventually include several strategic partners:

- Universities (e.g., IIT, Iowa State, Princeton, Texas A&M, San Diego State, U. Colorado ...): Develop accurate models, numerical techniques, high-end computing methods, and visualization techniques. Collect lab-scale experimental data. Organize technology focused workshops and conferences.
- Research groups at other National Labs (e.g., ORNL, ...): Develop advanced computational components and techniques.
- Software/Engineering businesses and research organizations (e.g., PSRI, Fluent, PSC, REI, ...): Develop software and models. Collect lab and pilot-scale experimental data. Develop methodologies for applying the models to solve technical problems. Transfer the computational technology to commercial codes.
- Technology Developers (e.g., KBR, Southern, Alstom Power, ...): Guide the development of a computation-assisted design methodology and adopt it for the design of future power plants.

Key Barriers:

The key barriers to launching the effort are securing the funding and organizing the collaboratory. Once the collaboratory is formed the key barriers to success can be classified into two groups:

- Process
    - Coordinating the development of models and experiments would involve changing the current practice of planning and executing projects.
    - Negotiating with the technology partners so that their proprietary data are protected without compromising the ability to expand engineering science knowledgebase.
    - A systematic outreach effort will be needed to gain the confidence of power plant designers in the use of computational technology.

- Technical
    - Fidelity of models, especially to describe complex industrial systems, needs to be improved.
    - The speed of computational models needs to be increased.
    - Need to develop methodologies to combine phenomenology (based on pilot plant data) and computational models.

  - Making measurements in dense gas-solids systems is technically challenging.

Indicators of Success:

The ultimate indicator of success would be the widespread adoption of the computation-assisted design methodology for the design of future power plants and consequent increase in the success of novel plant concepts. A concomitant indicator is world-wide recognition of CMFR as a center of excellence. These are expected in the tenth year of operation of the collaboratory. Some early indicators of success are outlined below:

During the seven to ten year time frame we expect to achieve the following:
- Computation-assisted invention of a new device
- Adoption by industry of computation-assisted design methodology
- Documented improvement in the design of a device

Starting from the fifth year we expect to have a significant increase in the following:
- Citation count of CMFR published papers
- Number of technology specific solutions
- Number of users of CMFR resources

Starting from the third year we expect to have a significant increase in the following:
- Number of papers published suitably normalized by the funding
- % of papers in high impact journals
- Speed and accuracy of the models
- Comprehensiveness of the library of models
- Experimental capabilities
- Number of collaborators
- % of external funding
- Number of joint experimental and modeling projects

References:

1. B.J. Ennis, J. Green, R. Davies, “The Legacy of Neglect in the U.S.,” *Chemical Eng. Progress*, 32-43, April 1994.
2. E.W. Merrow, “Linking R&D to Problems Experienced in Solids Processing,” Chemical Eng. Progress, 14-22, May 1985.
3. S.J. Clayton, G.J. Stiegel, and J.G. Wimer, “U.S. DOE’s Perspective on Long-Term Market Trends and R&D Needs in Gasification,” 5th European Gasification Conference: Gasification – The Clean Choice, Noordwijk, The Netherlands, April 8-10, 2002.
4. Clean Coal Technology Fact sheets (http://www.netl.doe.gov/cctc/summaries/fs_loc.html#indiana)
5. T.M. Knowlton, S.B.R. Karri, A. Issangya, “Scale-up of fluidized-bed hydrodynamics,” Powder Technology, **150**, 72–77, 2005.
6. D. L. Davidson, “The Role of Computational Fluid Dynamics in Process Industries” *The Bridge* (National Academy of Engineering), Volume **32**, Number 4 - winter 2002.
7. Chemical Industry of the Future. Technology Roadmap for Computational Fluid Dynamics, October 1997.
8. NETL Institutional Plan FY 2003-2007

Appendix A: Existing Capabilities at NETL

Gas-Solids Flow Experimental Facilities

The Cold-Flow Circulating Fluidized Bed (CF-CFB) in Morgantown is an industrial scale cold model. The riser is constructed of flanged steel sections with several 1.22-m acrylic sections capable of operating up to 4 atmospheres. A schematic is shown in Figure 1. The solids enter the riser through a non-mechanical valve located directly above the gas distributor. A loop-seal is depicted in Figure 1, but we have also tested L-Valve, J-Valve, and N-valve configurations. Solids exit the riser about 1-m below the top, are captured by the primary cyclone and returned to the riser through a 0.25-m diameter standpipe and a non-mechanical valve. Fine particles escaping the primary cyclone are collected by a secondary cyclone and a bag house. Gas velocities, pressure, temperature, and humidity are actively controlled. The primary response measurement was the overall riser pressure differential; it was calibrated within 0.45 Pa/m. The mass circulation rate is continuously recorded by measuring the rotational speed of NETL's unique, twisted spiral vane located in the packed bed region of the standpipe. The circulation rate can be actively controlled to a set-point using feedback from the spiral solids flow meter to adjust the aeration to the standpipe.

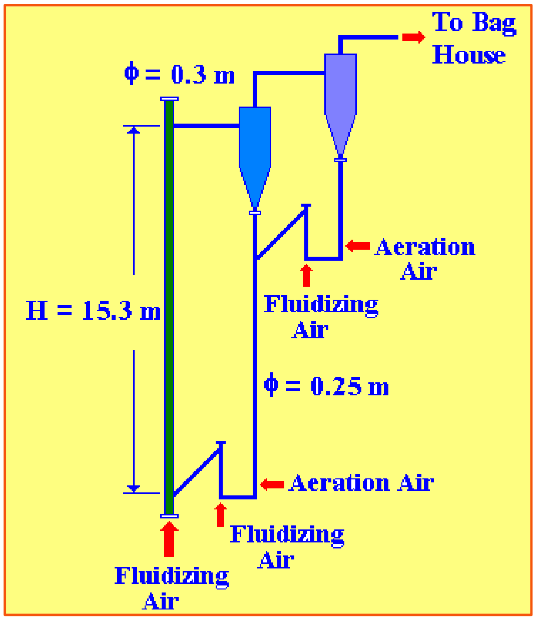


Figure 4. Schematic diagram for the 0.3 m diameter circulating fluidized bed cold flow facility

The key features and advanced measurement capabilities of the facility are summarized below:

- Riser: 15.45 m (height) x 0.305 m (diameter)
- Standpipe: 11.4 m (height) x 0.23 m (diameter)
- Advanced Research Measurements:
    - Solid Circulation Rate:
        - Spiral meter
        - Transient solids cutoff methods
    - Gas and Solids Velocity :
        - Laser Doppler Velocimeter (LDV)
        - Fiber optic probe – Vector probe
        - REM probe – refined fiber optic probe
        - Tracer gas pulse injection

        - Anemometer
    - Solid Concentration Measurements:
        - △P measurement - pressure transmitters (22 in riser alone)
        - Optical transmission probe - local
        - Densitometer average bed density
        - 3D Capacitance Imaging System
    - Solid and Gas Mixing and Mass Transfer
        - Pressure fluctuations – turbulence intensity
        - Gas tracer and sampling probes
        - Solids tracer and sampling probes
- Maximum Riser Superficial Gas Velocity: 10 m/s
- Maximum Solid Flux: 380 $kg/m^2 \cdot s$

The unit has been tested over a wide range of operating regimes from turbulent flow up to dilute up-flow transport. The variables tested include riser velocity, solids circulation rate, standpipe and non-mechanical aeration rates, riser pressure, total system inventory, and particle size and density. Various CFB configurations, including solids separators and non-mechanical valves, have also been tested. Over the past 5 years the results have been published in a number of reports describing the development of advanced instruments and methods, the characterization of various operating regimes, the assessment of various process applications, the evaluation and development of engineering relationships, the development of dynamic models and controls, and validation of computational fluid dynamic models.

Larger scale process studies can be conducted in a sorbent circulation loop of an abandoned section of the Modular CO_2 Capture Facility (MCCF), formerly known as the Life-Cycle Test System (LCTS). NETL had designed, constructed, and operated the LCTS. It was used primarily for the investigation of dry, regenerable sorbent flue gas cleanup processes. Sorbent was continuously cycled from an absorber reactor, where the pollutants were removed from the flue gas, to a regenerator reactor, where the activity of the spent sorbent was restored and a usable by-product stream of gas was produced. The LCTS evaluated the Moving-Bed Copper Oxide Process by determining the effects of various process parameters on SO_2 and NO_x removals.

The LCTS is located on the east side of the highbay of Building 84; it is the first project to be operated in this highbay. The process is housed in a structural steel frame composed of three levels with open grating floors. The levels are connected by two stairwells, each with handrails. A catwalk connects the fourth level to a south exit door into a transition area to provide alternative means of egress (less than 75 ft) from the platform. A 12-ton overhead crane services the building. Since the process investigated used a reducing gas and an oxidizing gas in a sorbent looping process, a SARS of the highest level was obtained for this unit.

The LCTS facility can be subdivided into two process functions: production and subsequent treatment of the flue gas, and sorbent transport and processing. The sorbent process stream involves a closed-loop cycle of sorbent transported through four major vessels. The sorbent absorbs flue gas contaminants in an absorber, passes through a fluidized-bed sorbent heater where it is heated with air and the products of a natural gas combustor, enters a regenerator where it is treated with a reducing gas (natural gas or methane) and gaseous sulfur-containing species are released, and passes through a fluidized-bed air cooler prior to returning to the absorber. The sorbent is gravity fed through all four vessels, with the exception being the line connecting the absorber exit with the fluidized-bed sorbent heater. In this line, a pneumatic transport system sends the sorbent to an elevated location (i.e., the sorbent heater) to repeat the gravity-fed sorbent cycle. The hot air from the sorbent heater is vented through a baghouse for dust removal, and the regenerator offgas is vented through an incinerator.

The entire system operates at pressures close to ambient; the various vessel pressures are maintained by forced draft and induced draft blowers and control valves. Currently, the sorbent system can operate at temperatures ranging from 700 to 1100^{o}F. The absorber and regenerator have externally mounted heaters for temperature maintenance. Sorbent flows were in the range 0.5 to 3 lb/min.

The Gas Process Development Unit (GPDU) is a proof-of-concept-scale facility designed to evaluate solid metal-oxide sorbents for removal of sulfurous compounds from a gasification-based syngas at pressures up to 385 psig and temperatures up to 1200 °F. The facility includes two fluidized-bed reactors (18” i.d. x 10’ deep and 10” i.d. x 12’ deep), and two transport reactors (5.2” i.d. x 50’ long and 1.7” i.d. x 50’ long). These four reactors can be coupled in four different configurations to provide continuous gas processing with a solids reduction reaction occurring in one reactor and a solids oxidation reaction occurring in the other reactor: 1) transport reactor and transport reactor, 2) fluidized-bed reactor and fluidized-bed reactor, 3) transport reactor and fluidized-bed reactor, or 4) fluidized-bed reactor and transport reactor. The existing facility includes the infrastructure to evaluate catalyst performance and solid-gas flow properties at temperatures, pressures, and flow rates at a scale that will reasonably estimate commercial scale facility/process performance.

Solid-Gas Flow Simulation Capabilities

Two computer codes are used extensively at NETL to simulate gas-particles flows, the Open-Source code MFIX and the commercial code FLUENT. The first code, MFIX (**M**ultiphase **F**low with **I**nterphase e**X**changes), is a general-purpose computer code developed at NETL for describing the hydrodynamics, heat transfer and chemical reactions in heavily-loaded, fluid-solids systems. It has been used for describing bubbling and circulating fluidized beds and spouted beds. MFIX calculations give transient data on the three-dimensional distribution of pressure, velocity, temperature, and species mass fractions. MFIX code is based on a generally accepted set of multiphase flow equations. The code is used as a "test-stand" for testing and developing multiphase flow constitutive equations. Some of the features of MFIX are:

- Mass, momentum, energy and species balance equations for gas and multiple solids phases
- Granular stress equations based on kinetic theory and frictional flow theory
- Three-dimensional Cartesian or cylindrical coordinate systems with nonuniform mesh size
- Impermeable and semi-permeable internal surfaces
- Set up the simulation with an input data file
- Define chemical reactions and kinetics with the input data file or with a user-defined subroutine
- Error checking of user input
- Multiple, single-precision, binary, direct-access output files that reduces disk space and increases data retrieval speed
- Post-processing codes for the animation and retrieval of output data
- Fortran 90 code base with allocatable arrays
- Generate serial, shared-memory parallel (SMP) or distributed-memory parallel (DMP) executables from the same code base

This MFIX code is distributed through the web site http://www.mfix.org. It has been downloaded by over 500 researchers from over 200 institutions all over the world. It is actively being extended and used for research at NETL, ORNL and at several external research groups around the world. Currently, MFIX developers at different sites contribute to and communicate advances in this simulation package. Source-code modifications are managed using version control software, so that each change is documented. New versions are tested against a suite of control cases.

The second code, the FLUENT code, is the world leading CFD code for a wide range of flow modeling applications. It is very user-friendly, making it easy for new users to come up to productive speed very rapidly. Its unique capabilities in an unstructured, finite volume based solver are near-ideal in parallel performance. It has been put through a comprehensive program of verification testing to ensure that FLUENT is ready to deploy right out-of-the-box. The general modeling capabilities of FLUENT include:

- Complete mesh flexibility
- All speed regimes (low subsonic, transonic, supersonic, and hypersonic flows)
- Parallel processing
- Solution-based mesh adaption
- Steady-state and transient flows
- Inviscid, laminar, and turbulent flows
- Newtonian or non-Newtonian flows
- Full range of turbulence models from simple k-epsilon models to large eddy simulation (LES)
- Heat transfer including forced, natural, and mixed convection, conjugate heat transfer, as well as several radiation models
- Chemical species transport and reaction, including homogeneous and heterogeneous combustion models and surface reaction models
- Free surface, Eulerian and mixture multiphase models
- Lagrangian trajectory calculation for dispersed phase modeling (particles/droplets/bubbles)
- Phase change model for melting/solidification applications
- Cavitation model
- Porous media model
- Lumped parameter models for fans, radiators, and heat exchangers
- Dynamic mesh capability for modeling flow around moving bodies
- Inertial (stationary) or non-inertial (rotating or accelerating) reference frames
- Multiple reference frame and sliding mesh options
- Mixing-plane model for rotor-stator interactions
- Acoustics analogy for prediction of flow-induced noise
- Materials property database
- Integrated problem set-up and post-processing
- Extensive customization via user-defined functions

Appendix B: Tentative CMFR Plans

The Collaboratory for Multiphase Flow Research — CMFR — organizes research related to multiphase flow that has applications in the power and process industries. It is jointly sponsored by the National Energy Technology Laboratory, West Virginia University, University of Pittsburgh and Carnegie Mellon University.

Mission:

- Develop multiphase flow models and numerical techniques
- Validate the models with well calibrated experiments
- Promote the use of computational tools in industrial practice
- Provide a focal point for collaboration with academic and national labs
- Disseminate information and attract young researchers to the subject

Activities:

- Develop and maintain a long-range multiphase research plan to support the NETL/DOE mission.
- Coordinate research projects by a CMFR Executive Committee and annually review the projects by a Technical Advisory Board.
- Infrastructure development
    - Software
    - Hardware
    - Personnel
- Outreach activities: CMFR website; sponsorship of short and long term projects by graduate students, faculty and postdoctoral fellows; organize technical talks, conferences, and workshops.
- Promote the awareness, acceptance, and implementation of CMFR through direct and indirect technology transfer, technical assistance, promotional initiatives, training, and participation in research activities.

List of Research Topics:

- Analysis of technology barrier issues and how combined modeling and experiments can be used to address the challenges
- Increasing the speed of simulations so as to make impact on experimental campaigns and design and troubleshooting efforts.
- Making suitable experimental measurements and developing models that combine phenomenology with fundamental science
- Consideration of variability in the input data to models
- Developing a protocol for validating models using data from pilot-plants
    - Uncertainties in measurements
    - Data reconciliation to solve mass/energy balance problems
    - Pilot plants not reaching steady state
- Development of a consistent hierarchy of models ranging from detailed CFD to simpler reduced-order-models (ROM).

- Extraction of information useful for design and analysis from the results of CFD and other model simulations.
- Communication of simulation results to design engineers.

Timeline:

- Conduct internal discussions at NETL – 3-4/2005
- Obtain Internal approval – 5/2005
- Complete an internal whitepaper on CMFR at NETL -- 6/2005
- Incorporate local universities – 10-11/2005
- Invite external participants to CMFR – 11/2005 – 1/2006
- Complete the CMFR charter incorporating comments from external participants -- 3/2006
- Conduct a "collaboratory forming" kick off meeting --4/2006
- Develop a start up budget for the first five years of the collaboratory's operation – 5/2006
- Secure funding for the collaboratory – 7/2006
- Establish the Executive Committee and Technical Advisory Board of the collaboratory – 9/2006
- Plan research projects and launch the collaboratory -- 10/2006