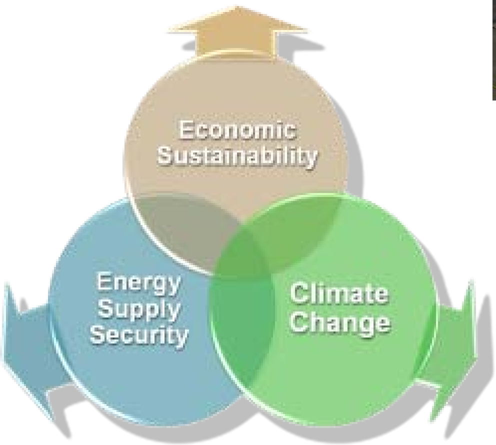
NATIONAL ENERGY TECHNOLOGY LABORATORY



Overview of National Energy Technology Laboratory R&D Activities and Partnership Opportunities

Chris Guenther[1], J. Bennett, M.Shahnam, D. VanEssendelft, E. Granite, and S. Zitney

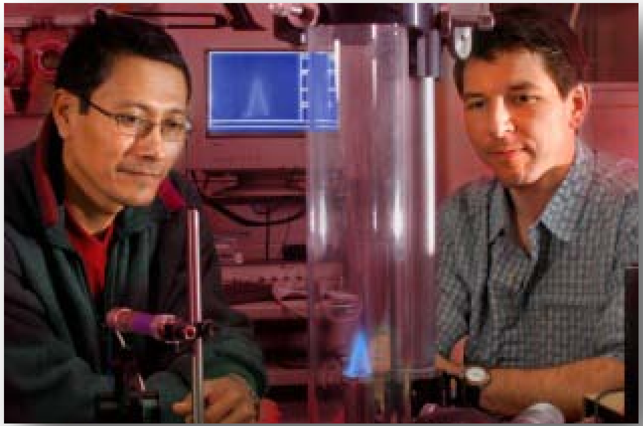
National Energy Technology Laboratory (NETL)

[1]Team Technical Coordinator, NETL Gasification Team and Director of the Computational Science Division

Gasification Technologies Conference, Oct. 9th-12th 2011 San Francisco, CA

Agenda

- **NETL's Gasification Team Tasks**
  - Refractory Improvement
  - Conversion and Fouling
  - Low Rank Coal Optimization
  - Warm Gas Clean-up
  - NETL's IGCC Simulator and Training facility
- **Questions**



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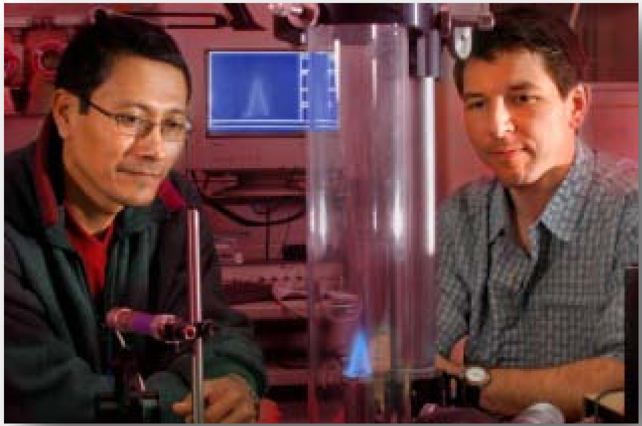
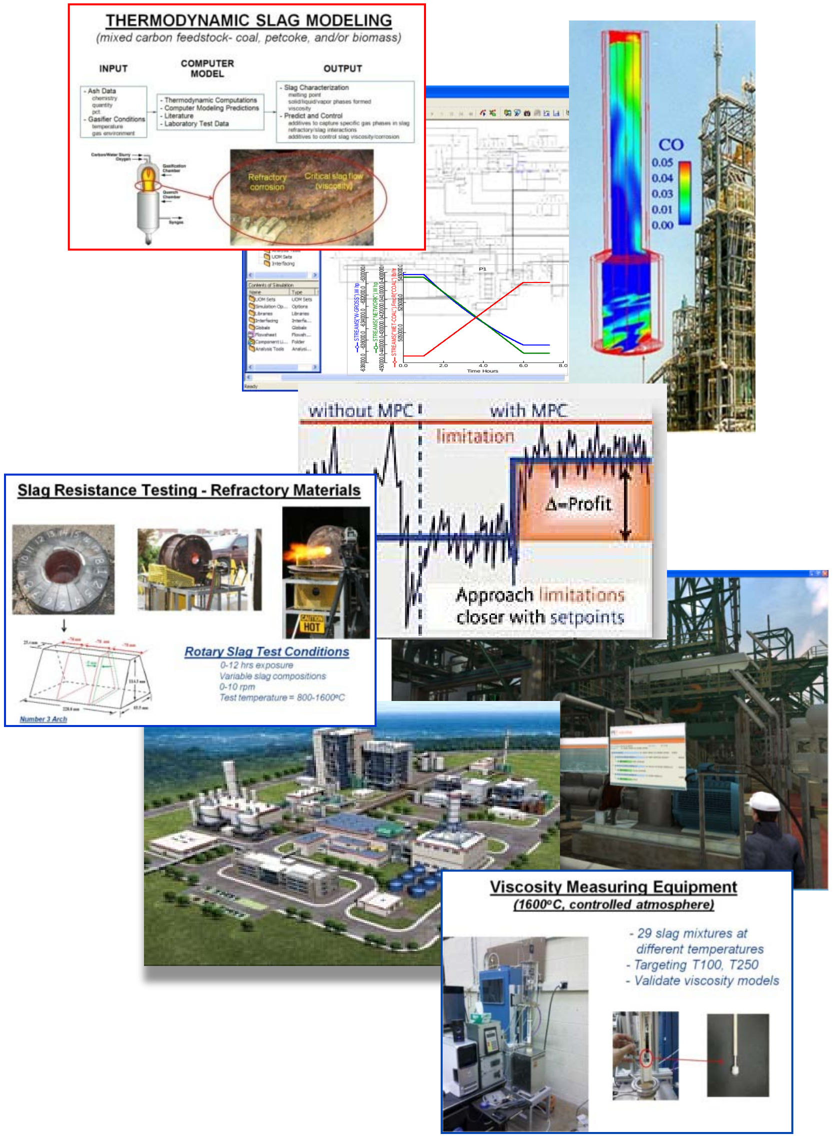


Gasification Team



Gasification Team Goal:

To use an integrated approach which leverages on-site support and regional university partners to combine theory, computational modeling, experiment, and industrial input to develop physics-based methods, models, and tools to support the development and deployment of advanced gasification based devices and systems.

Gasification Team Task Structure

Gasification Team (Guenther)

	Refractory Improvement	Conversion & Fouling	Low Rank Coal Optimization	Warm Gas Clean-up	AVESTAR Center
Tasks	Refractory Improvement	Conversion & Fouling	Low Rank Coal Optimization	Warm Gas Clean-up	AVESTAR Center
Task Mission	*Improved capacity Factor for lower COE*	*Higher efficiency by enabling syngas heat Recovery without fouling*	*Enable low-rank coal and mixed feed gasification performance prediction and improvements*	*Back-up option To meet EPA trace metal rules*	*Develop IGCC Training Strategy and Approach.*

Existing bituminous application — *Low-rank & mixed feedstock* — *Both*

NETL, URS, and Regional University Alliance FTE Allocation

NETL/ORD	CMU	PSU	WVU	URS	Industrial Collaborators
17	3	3	3	12	5

Task – Refractory Improvement

Goal:

- *Refractory liners = develop liners that are carbon feedstock flexible (coal, western coal, petcoke) with improved performance*
- *Model gasifier slag = refractory interactions, viscosity, downstream phases and material interactions (syngas coolers)*
- *Manage slag viscosity and refractory wear, evaluate additives*

Overall Objectives:

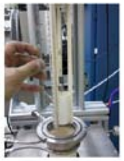
- *Increase gasifier RAM (Reliability, Availability, Maintainability)*
- *Develop gasification as a fuel and product flexible energy conversion system competitive with conventional pulverized coal power plants*

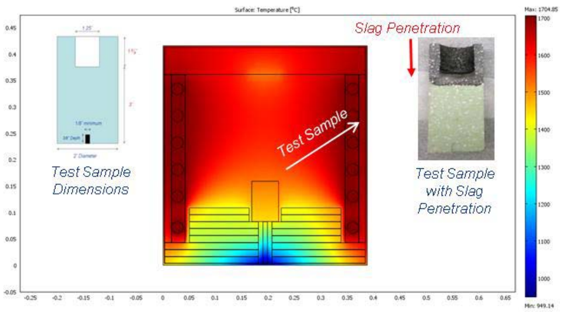
Task	FY12 Objectives
Refractory Improvement	• *Determine critical information for slag management for gasifiers* • *Analyze data and samples related to wear, chemistry, viscosity, and phases for modeling* • *Vanadium temperature/O2 partial pressure phase studies* • *Determine mechanism of wear in NETL refractory materials under development* • *Determine refractory corrosion mechanisms in current generation commercial refractory liner materials exposed to coal slag.*

FY 2011 Program Accomplishments

- **Petcoke contains vanadium at high levels. Behavior of vanadium oxide in gasification environments established.**
- **Cr^{+6} formation in gasifier refractory linings shown thermodynamically not to occur at levels of concern in current carbon feedstock.**
- **Approaches to slag management for controlling solid-liquid-gas phases originating in carbon feedstock mineral impurities have accurately predicted refractory corrosion - slag modeling and control underway to increase gasifier RAM.**

Viscosity Measurements
(1600°C, controlled atmosphere)

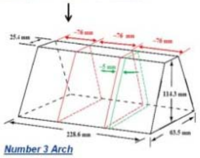




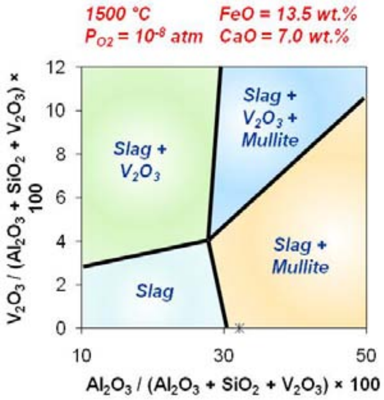
Thermal Profile of Refractory Sample in Test Furnace

High Temperature TGA
(1600°C, controlled atmosphere, up to 100 gm sample)

Slag Resistance Testing - Refractory Materials

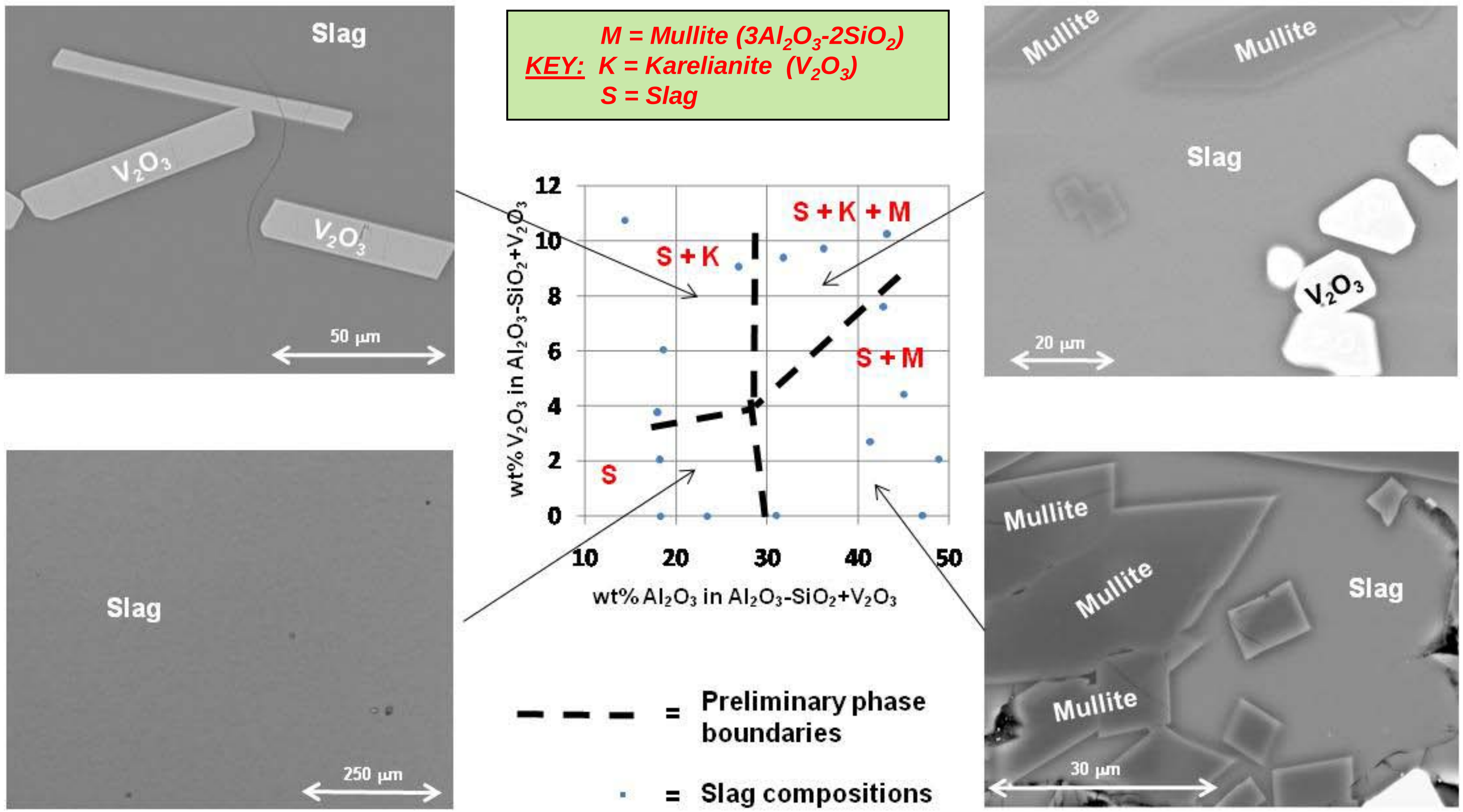


Rotary Slag Test Conditions
0-12 hrs exposure
Variable slag compositions
0-10 rpm
Test temperature = 800-1600°C



Preliminary Phase Equilibrium Established for Petcoke/Slag Synthetic Mixtures

(impacts slag flow, refractory wear)



Phase diagram represents 13.5 wt pct FeO, 7 wt pct CaO, and variations of SiO_2, Al_2O_3, and V_2O_3. Temp = 1500°C, O_2 partial pressure of 10^{-8} atm, 72 hr soak.

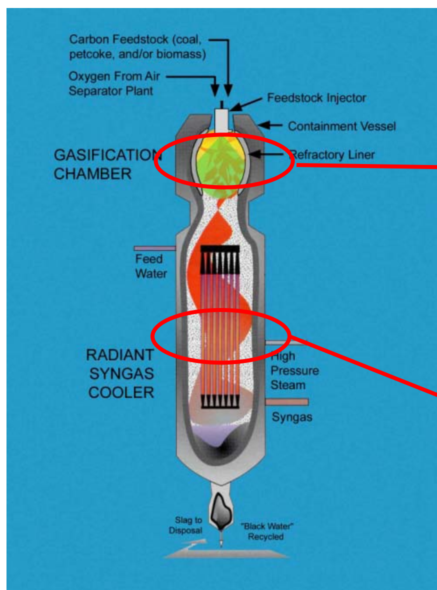
Note: Confirming phase equilibrium results in commercial gasifier slags, expanding gasifier conditions in FY 12

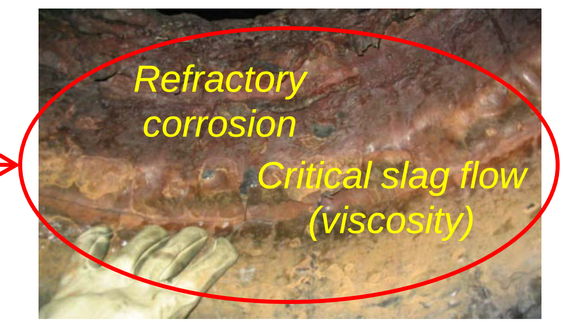
Current Program Emphasis – Slag Management *(mixed carbon feedstock- coal, western coal,*

INPUT	COMPUTER MODEL	OUTPUT
- Ash Data chemistry quantity pct. - Gasifier Conditions temperature gas environment	- Thermodynamic Computations - Computer Modeling Predictions - Literature - Laboratory Test Data	- Slag Characterization melting point solid/liquid/vapor phases formed viscosity - Predict and Control additives to capture specific gas phases in slag refractory/slag interactions additives to control slag viscosity/corrosion

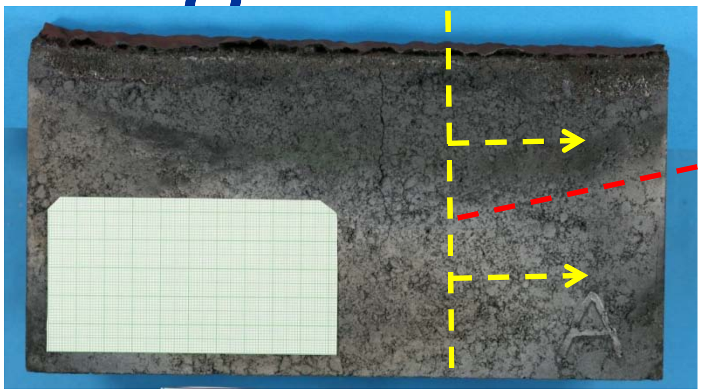
GOALS

- ***Primary*** *- control refractory wear and slag flow*
- ***Secondary*** *-* minimize syngas cooler fouling





High Cr_2O_3 Refractory Material Development
(Patent Application S-122,347 Filed on 4/7/2011)

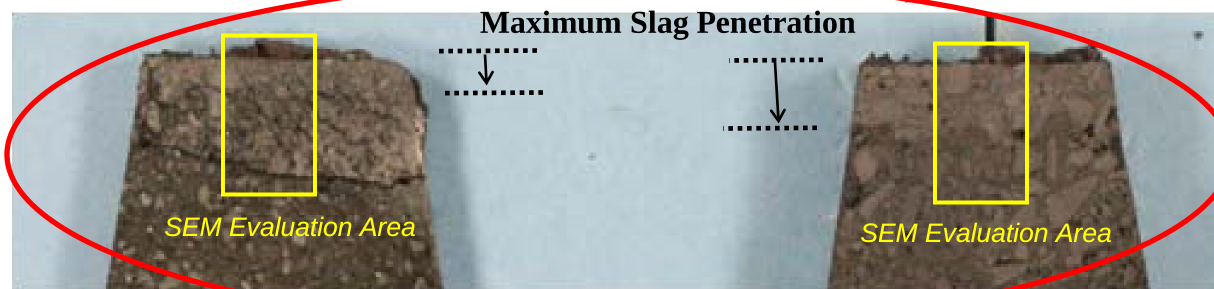


Rotary Slag Test Sample

Cross Section

Slag contact (hot face)

No slag contact (cold face)



Modified | **Not Modified**

Sample area used for SEM microstructure analysis

Test used to determine samples with potential for gasifier application

Refractory/Slag Interaction

Sample	Distance Removed (mm)*	Visual Slag Penetration Depth (mm)
High Cr_2O_3 Not Modified	1.3	4.3
High Cr_2O_3 Modified	0.8	1.8

Current refractory goal is to refine/evaluate composition in commercial gasifiers

Refractory/Slag Program Needs

Current Refractory Program Needs

Materials/Samples

- Slag feedstock chemistry ranges and slag flow characteristics
- Gasifier target conditions for slag modeling/management
- Samples of spent slag, refractory materials (liner, thermocouple assemblies), downstream syngas fouling

NDA/CRADA Agreements

- Eastman Chemical
- ConocoPhillips
- Need additional cooperators for slag modeling/ management, refractory development, and gasifier material samples

Contact Information

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Task – Conversion and Fouling

Goal:

- *Higher efficiency and capacity factor by enabling syngas heat recovery without fouling.*
- *To collaborate with industry to ensure proper technology development and transfer*

Overall Objectives:

- *Develop reduced-order and detailed models to address syngas fouling issues for entrained flow gasifier system, based on initial grind and coal preparation.*
- *Conduct laboratory experiments to provide model data for devolitization, char gasification kinetics, and ash deposition.*
- *Test and validate methods/predictions of reduced fouling.*

Task / Activity	FY12 Objectives
Conversion and Fouling 1. Modeling 2. Kinetics (kinetics and ash formation) 3. Slag Characterization 4. Particle Deposition	• Predictions of the slag-flyash split using the initial heuristic spreadsheet-based reduced-order model (ROM) for entrained-flow gasifiers will be evaluated for Pittsburgh #8 coal. • Complete pyrolysis and gasification kinetic measurements for various density and size fraction of Pittsburgh #8. • Determine the viscosity for 2 synthetic coal slags (eastern and western). • Design and modify the existing NETL reactor to accommodate particle deposition experiments.

Conversion and Fouling: Modeling

<u>Goals</u>: To determine effects of various coal and/or Petcoke fuel properties (for various density and size fractions) on unconverted carbon and syngas cooler fouling in entrained flow gasifier systems. Develop and validate two spreadsheet models: a heuristic model based on an existing spreadsheet model for Bailey Coal, and a second higher-fidelity model that will allow CFD results to be used as input.

<u>Recent accomplishments</u>: Over the past year, various particle deposition models have been evaluated and the results have been documented in two papers:

1.) W. Ai and J. M. Kuhlman, *Energy and Fuels* 25, 708-718, Feb. 2011.

2.) J. M. Kuhlman and W. Ai, 28th Int'l. Pittsburgh Coal Conference, Pittsburgh, PA, Sept. 2011.

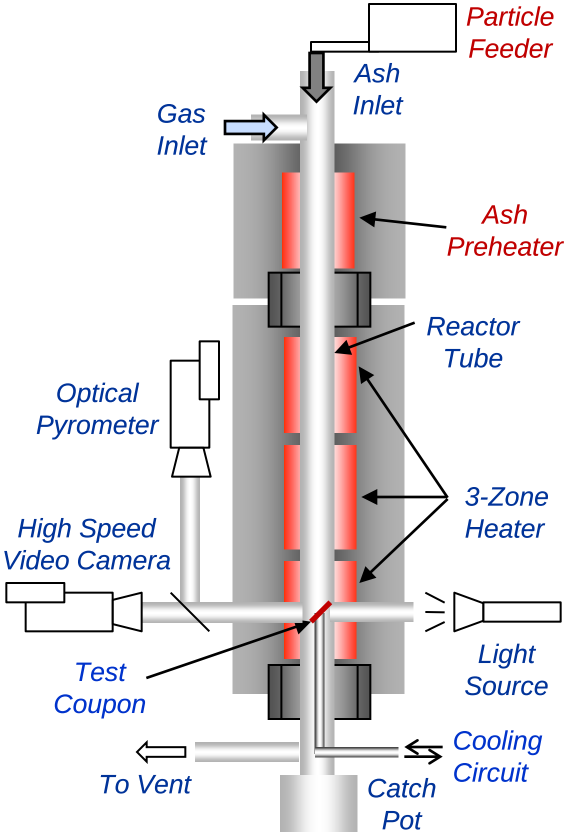
<u>2012 Objectives and Plans:</u>

1.) Evaluate & validate submodels for particle-slag interaction, particle fragmentation, and mineral matter chemistry (sulfur release) and implement into CFD model.

2.) Develop and evaluate heuristic spreadsheet-based reduced order model (ROM) to predict mineral matter split between slag and flyash for entrained-flow gasifier.

Conversion and Fouling: *Convective Syngas Cooler Fouling*

- **<u>Goals</u>: Relate ash particle deposition to feedstock & flyash properties, surface temperature & geometry, and flow properties**
  - Provide empirical data to the modeling taskto enable CFD/Reduced Order modeling of CSC fouling
  - Study effect of additives and FeS on ash deposition/agglomeration
- **2012 Objectives and Plans**
  - Literature survey of deposition models
  - Modify high pressure tubular reactor at NETL for ash deposition studies
  - Investigate gasifier ash deposits to determine problematic ash characteristics

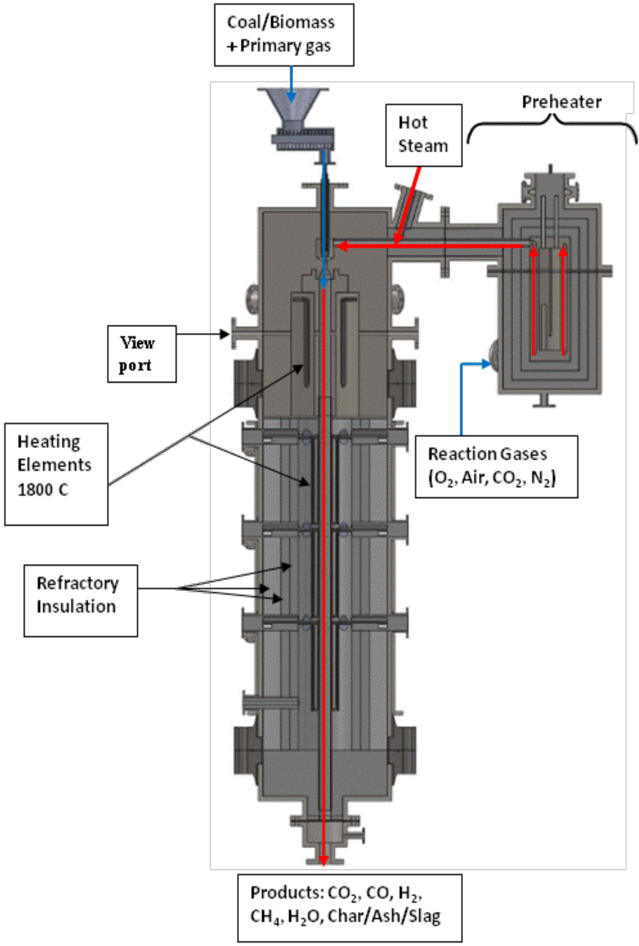


WestVirginiaUniversity

Conversion and Fouling: *Kinetics*

Goal: Ash forming mechanisms in a high pressure entrained flow gasifier are not available. Heterogeneity of coal shadows the ash forming mechanisms and therefore a wide range of particle size and density fractions of coal is selected for this research.

- Characterize physical changes and chemical changes
- Determine the extent of fragmentation/coalescence of ash at various char conversions by evaluating the residual particle size distributions.
- Determine the critical conversion at which char fragmentation occurs, chemical transformation of excluded minerals to ash/slag at various residence times, and the physical transformation of excluded minerals to ash/slag at various residence times.



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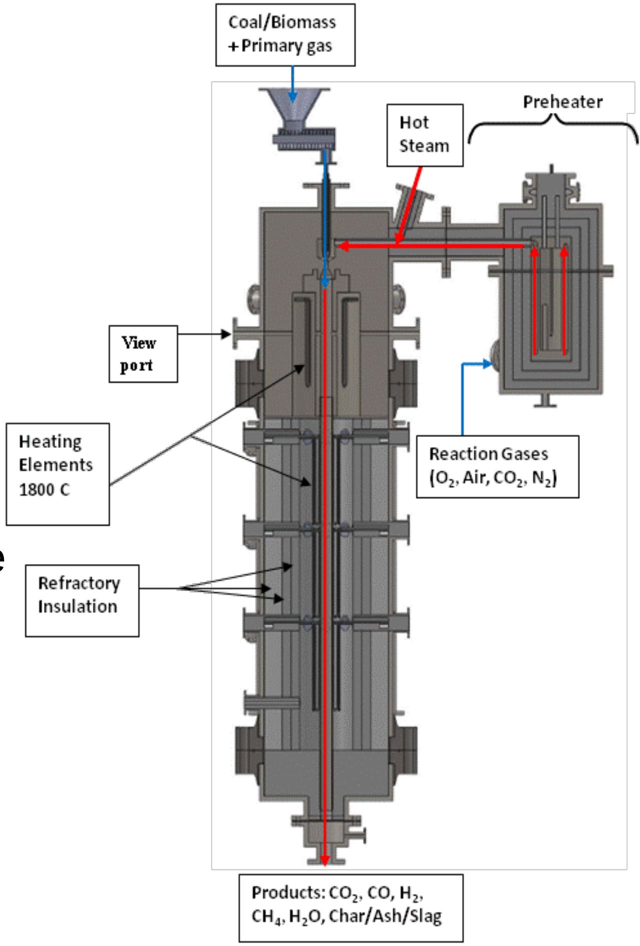
Conversion and Fouling: *Kinetics*

- **FY12 Objectives and Plans**
  - Effect of Pressure on Pyrolysis Kinetics
    - 24 tests performed at 20 and 30 atm.
    - Characterize generated chars and ashes for morphology particle size distribution, density, ash phases and ash composition.
  - Preliminary Gasification kinetics at high pressure
    - 4 density cuts and 2 size fractions char samples from Pitt# 8 coal will be gasified at 1300, 1400, and 1500 C under CO2 and H2O atmosphere in the High Pressure Entrained Flow Reactor (HPEFR). Perform necessary characterization, such as density, internal surface area, morphology (SEM)
  - Gasification kinetics at high pressure (20 and 30 Atm)
  - Pyrolysis Kinetics of Pet Coke



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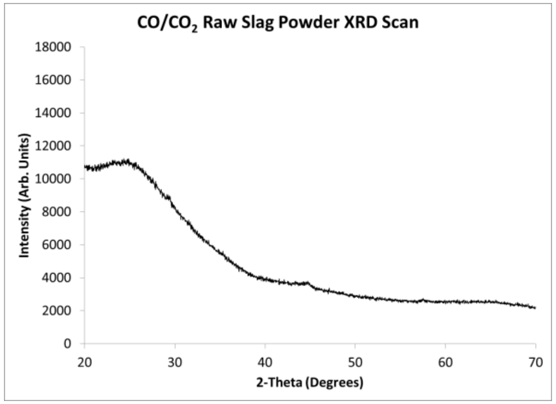
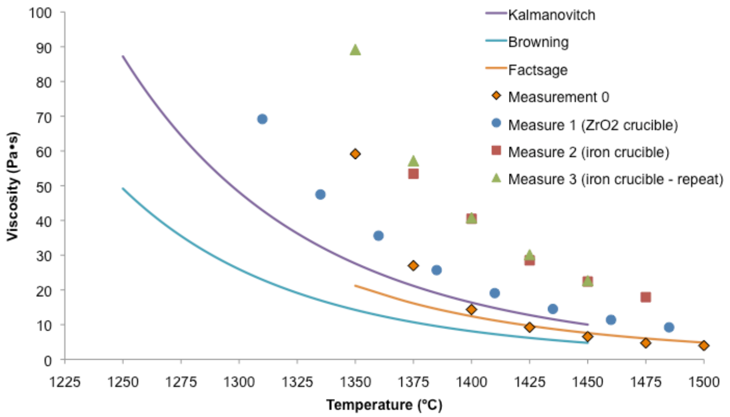
Conversion and Fouling: Slag Characterization

***Goal** – Slag generated from coal and coal/petcoke mixed feedstock, 1) characterize their crystallization behavior and viscosity, and 2) evaluate the behavior of slag FeS and VOx*

***Accomplishments to date** – Synthetic coal and coal/petcoke ash blends have had crystalline behavior, chemistry, and viscosity characterized.*

Coal Slag XRD Crystalline Phases (amorphorous)





	Al_2O_3	SiO_2	Fe_2O_3	CaO	MgO	Na_2O	K_2O	V_2O_3	NiO	P_2O_3	Total
wt%	26.3	45.5	17.8	6.1	1.3	0.9	1.5	0.0	0.0	0.7	100.1
at%	19.8	58.1	8.6	8.3	2.5	1.1	1.2	0.0	0.0	0.4	100

Coal Slag Chemistry

Coal Slag Viscosity Versus Temp (°C)

***2012 Objectives and Plans** – Continue to characterize coal/petcoke blends, characterize ash/slag generated by Penn State, begin studies of FeS and VOx behavior in slag.*

Carnegie Mellon

Conversion and Fouling: Collaborative Opportunities

- **Program Goal: In slagging gasifiers using coal, petcoke or mixtures of them; 1) improve the carbon conversion efficiency to syngas (reduce excess carbon), and 2) reduce convective syngas cooler fouling**

These issues impact plant efficiency; gasifier reliability, availability, and maintainability. They also place additional strains on solids handling and grey water circuits.

Source – Global Energy, Inc

NETL-RUA Conversion and Fouling Team		
Team Leader:	**Chris Guenther**	**NETL**
Slag and Fouling Modeling:	**John Kuhlman**	**West Virginia University**
Kinetic measurements:	**Sarma Pisupati**	**Penn State University**
Refractory and Slag:	**James Bennett and Sridhar Seetheraman**	**NETL Carnegie-Mellon University**
Particle Deposition:	**Nate Weiland and Nick Means**	**West Virginia University URS Corporation**

- **NETL seeks cooperators to improve carbon conversion and to reduce convective syngas cooler fouling.**

Task – Low Rank Coal Optimization

Goal:

•*Development of a hierarchy of co-feed TRIG models with uncertainty quantification (UQ).*

Overall Objectives:

- *Develop UQ framework into NETL's MFIX models*
- *Develop EE, EL, Hybrids, and ROM co-feed TRIG models.*
- *Conduct laboratory experiments to provide NETL's Carbonaceous Chemistry for Computational Modeling (C3M) data for char gasification kinetics.*
- *Incorporate torrefaction data into co-feed TRIG optimization studies*

Task / Activity	FY12 Objectives
Low Rank Coal Optimization 1. Model uncertainty quantification 2. Kinetics (PRB, eastern bit., and "woody" biomass 3. Hierarchy of co-feed TRIG models 4. Fuel Pretreatment	• Couple NETL's MFIX model to existing UQ models to determine model parameter sensitivity and perform UQ on large scale NCCC/TRIG • Development of hierarchy of co-feed TRIG models (E-L, EE, Hybrids, and ROM's) • Generate and analyze torrefied samples for energy content, composition, grindability, and lock-bridge feeder performance. • Generate gasification kinetic data and implement into NETL's C3M kinetic package

Low Rank Coal Optimization: Kinetics

Goal:

To investigate the kinetics and mechanisms of pyrolysis and gasification for mixed and low rank feedstocks to improve validate advanced gasification simulations

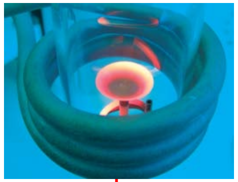
Experimental Approach:

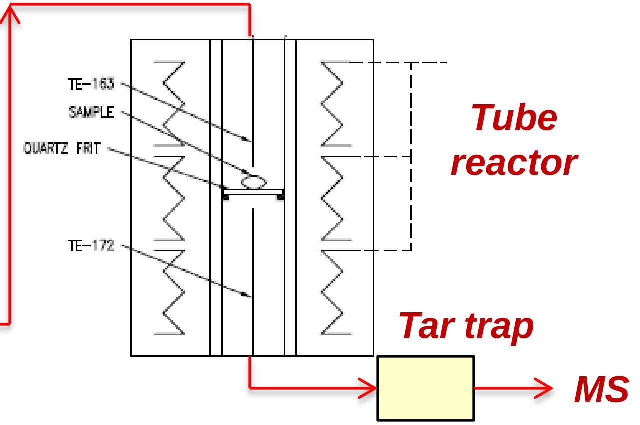
- **High Pressure Tubular Reactor**
- **Multi-functional TGA-Tube reactor-MS system**

2012 Objectives and Plans:

- **Baseline co-gasification kinetics for TRIG**
  - ✓ Study co-pyrolysis kinetics of PRB coal/wood blends
  - ✓ Determine char co-gasification kinetics in CO_2 and H_2
  - ✓ Modify the HTPR for char co-gasification in H_2O and O_2
- **Tar cracking kinetics**
  - ✓ Set up a TGA-Tube reactor-MS system
  - ✓ Determine tar generation rates
  - ✓ Initiate tar cracking rate study
- **Soot formation kinetics**
  - ✓ Modify the TGA-Tube reactor-MS system
  - ✓ Literature review and determine experiment matrix

HS-TGA





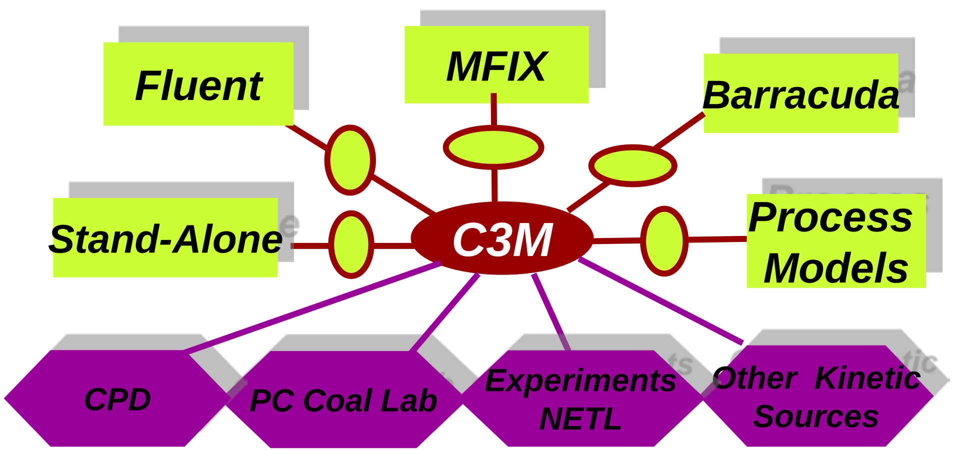
Low Rank Coal Optimization: Kinetics

Motivation

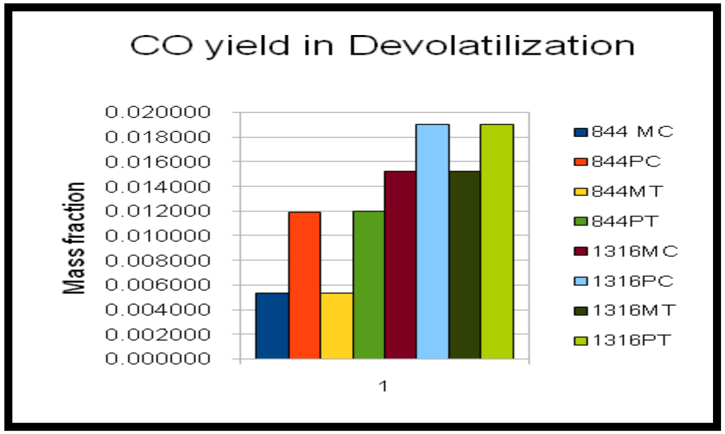
- *Currently kinetics information taken from literature needs to be reprogrammed for different CFD and process simulation software.*

Overall Goal

- *Develop software to bridge coal kinetics software (PCCL, CPD, etc) and available kinetic experiments with CFD software (MFIX, Fluent, Barracuda), other models and provide users with a virtual kinetic laboratory*



Architecture of C_3M



CO devolitization yields for 844 °C and 1316 °C from different kinetic sources

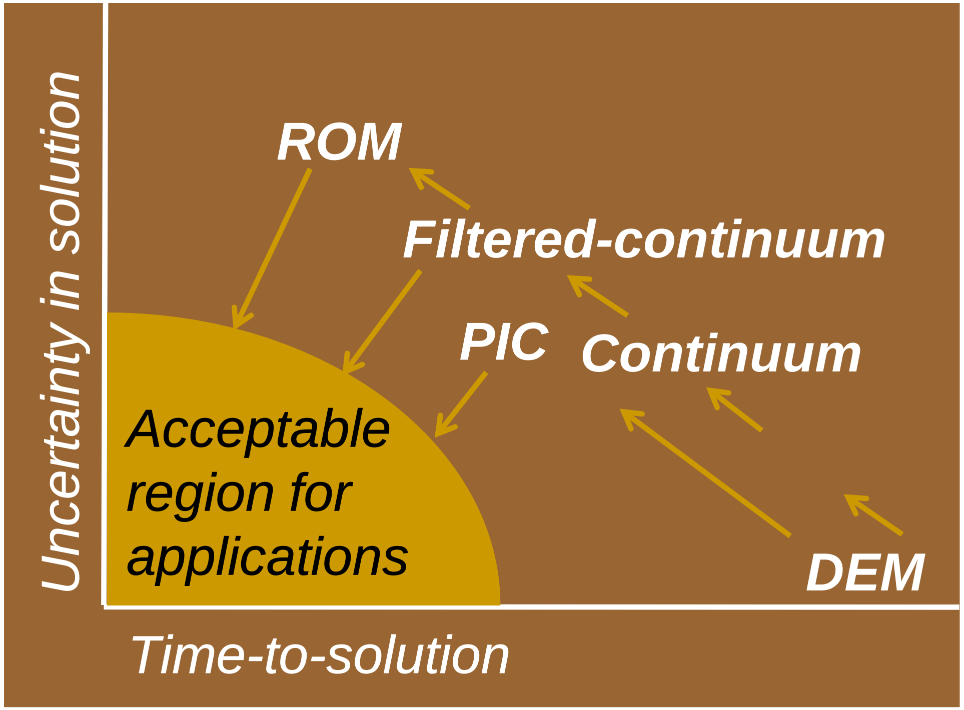
Low Rank Coal Optimization: Multiphase Models

Goal

- To develop an hierarchy of models for numerical simulations of gasifiers with a framework in place, to quantify the uncertainty associated with CFD characterization

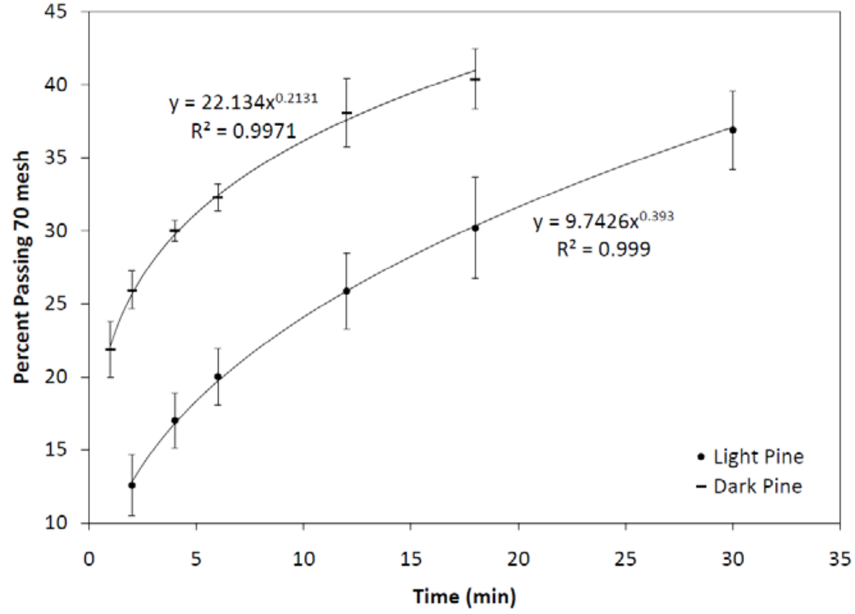
2012 Objective and Plans

- NETL's open source suite of multiphase solvers such as MFIX-DEM, MFIX continuum, MFIX-PIC and multiphase Reduced Order Models will be used to aid in the design and optimization of operating conditions and establishing performance trends in the NCCC/TRIG.



Reducing uncertainty and time-to-solution is the primary need in multiphase CFD

Low Rank Coal Optimization: Fuel Pretreatment



Goal

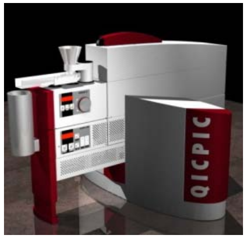
- Use the experimental fluid bed torrefaction system to optimize the torrefaction process conditions, generate materials for testing, and assess kinetics and energetics.

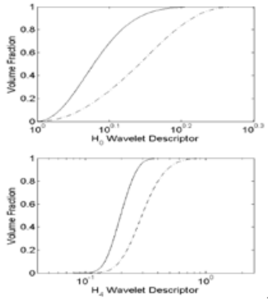
Recent Accomplishments

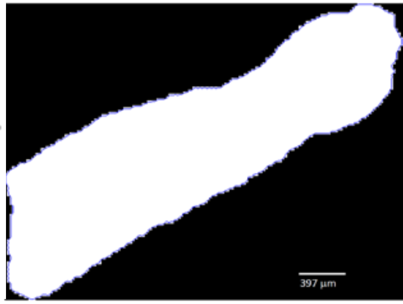
- Developed preliminary grinding laws based on two torrefied pine samples from NCSU
- Developed a computational method to very rapidly analyze particle shape contours which will help determine particle behavior in feeders and inter-phase physical forces in gasification models
- Completed first data sets on high confining stress solid mechanics which will allow us to model the feed systems computationally

2012 Objectives and Plans

- Expand and further test the grinding laws developed in FY11
- Correlate the NETL lab scale results with large scale grinding energies







- *Brought the QICPIC particle size and shape analyzer up to operational status*
- *Began collecting and analyzing data*
- *Will use the instrument and custom software to evaluate roughness and correlate to granular strength properties*

Task – Warm Gas Clean-up

Goal:

•Conduct both lab and pilot-scale R&D for cost efficient sorbents capable of meeting DOE and EPA targets for trace contaminant capture from coal gasification while preserving the high thermal efficiency of the IGCC system.

Overall Objectives:

- *Optimize palladium sorbents for Hg capture under development (loading and support)*
- *Conduct large scale Pd testing and cost analysis*
- *Conduct tests to investigate Pd sorbent capture of cadmium and antimony*
- *Sorbent based oxygen separation and hydrogen separation*
- *Investigate other sorbents*

Task / Activity	FY12
Warm Gas Clean-up	• Complete cost analysis and optimization of Pd sorbents for Hg capture • Conduct large scale Pd sorbent tests at relevant conditions.

Warm Gas Clean-up: Pd Sorbents for Hg

Motivation:

- EPA Announcement March 16, 2011 and National Rule by November 16, 2011
- Many States Requiring Mercury Removal
- >90% Removal Required – Existing Plants
- Higher Removal Levels – New Plants
- Maintain thermal efficiency

Recent Accomplishments

- Nearly 100% Removal of Hg, As and Se in Pilot Tests at 550ºF over Several Weeks
- Patent Issued April 2006
- CRADA with Johnson Matthey September 2005
- License with Johnson Matthey March 2007
- R&D 100 Award   October 2008

Task – IGCC Simulator and Training

Goal:

•Establish the world-class Advanced Virtual Energy Simulation Training and Research (AVESTAR^{TM}) Center for addressing the key operational and control challenges arising in advance gasification-based power plants with carbon capture.

Overall Objectives:

- *Develop, promote, market, and operate AVESTAR*
- *Improve plant wide IGCC regulatory and coordinated control strategies*
- *Develop load following strategies*
- *Develop advanced process control strategies for the IGCC dynamic simulator*

Task / Activity	FY12 Objectives
IGCC Simulator and Training	• Deploy immersive training system in AVESTAR • Develop, promote, market, and operate AVESTAR

AVESTAR™ Center at *Advanced Virtual Energy Simulation Training And Research*

Overview

- Objectives: Workforce training, education, and R&D on the efficient, safe, and reliable operation of clean energy systems
- Tools:
  - Real-time Operator Training Systems (OTS)
  - 3D virtual Immersive Training Systems (ITS)
- Simulators:
  - IGCC with CO_2 capture
  - Gasification / Combined Cycle
- Training:
  - Operations, Control, Startup, Shutdown
  - Load following, Malfunctions, Safety
- Facilities:
  - NETL, WVU/NRCCE in Morgantown, WV
- Customers: Utilities (eng, ops, trn, mgrs), E&Cs, Equipment vendors, Universities

Benefits

- Offers comprehensive training from introductory to advanced operations
- Provides integrated training for IGCC control room and plant field operators
- Enhances engineering education
- Affords opportunities for collaborative R&D in dynamics, control, safety, and 3D virtual technologies

Major Project Partners

NETL-RUA Regional University Alliance · West Virginia University · invensys · FCS Fossil Consulting Services, Inc.

Industry Collaborators

AEP · bp · DOOSAN · Great River Energy · Southern Company

IGCC Dynamic Simulator OTS/ITS
Capabilities and Features

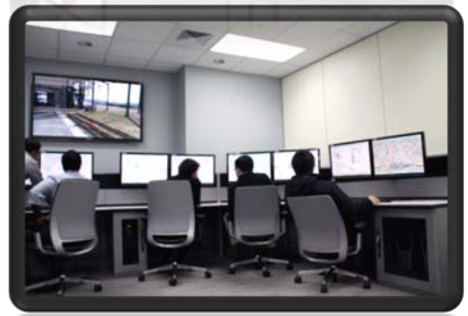
- Dynamic Simulator Scope
  - IGCC with CO_2 Capture
  - Fuel Switching and Co-firing
    - Coal, Petcoke, Biomass
- Model Fidelity
  - Mulitzonal kinetic reactor models
  - Startup, shutdown, load following
- Model Performance
  - Slow (0.5X), real-time, fast (2.5X)
  - Dynamic engines running in parallel
- OTS Features
  - Human-Machine Interface (HMI)
  - Variable and Group Trends
  - Audible and Visual Alarms
  - RFs, ICs, Malfunctions, Scenarios
- Process Controls
  - Regulatory PID control loops
  - Coordinated control
    - Gasifier and Gas turbine lead

- ITS Scope
  - 3D photorealistic virtual plant-wide model for IGCC with CO_2 Capture
  - Real-time integration with OTS
- 3D Immersive Interaction
  - Avatar represents plant field operator
  - Navigation/interaction using game pad
  - Projector/screen or LCD w/ 3D glasses
- 3D Virtual Content
  - Remote field functions, e.g.,
    - Manual valve turn
    - Pump switch on/off
  - Collision geometry and sound
  - Popup trends (variables vs. time)
  - Transparent equipment objects
    - Tanks, drums, heat exchangers
    - Distillation columns (e.g., CO_2 absorber)
    - Gasifier (slag flow, combustion/gasification)
  - Malfunction scenarios

AVESTAR Center Facilities

- **Locations**
  - NETL in Morgantown, WV
  - WVU, National Research Center for Coal & Energy
- **Facilities**
  - OTS Room: Control Room
    - Divider for 2 Simulators
  - ITS Room: Plant/Field
  - Local area network
- **Training Systems**
  - IGCC OTS
    - 8 Operator Stations
    - 2 Instructor Stations
    - 2 Engineering Stations
  - IGCC ITS
    - 2 Field Stations
    - 1 Instructor Station

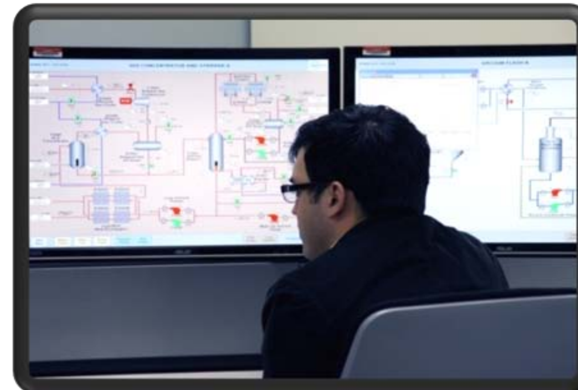
AVESTAR Center at NETL

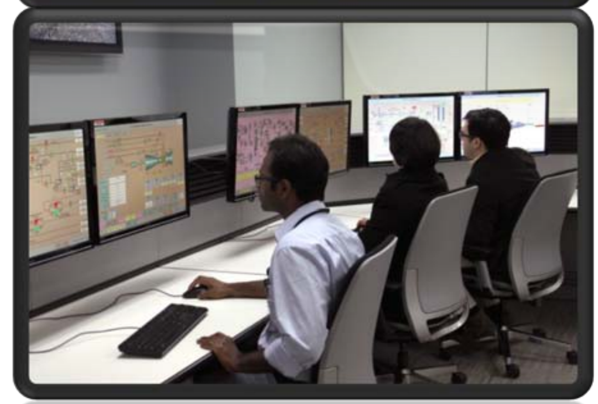


AVESTAR Center at WVU

AVESTAR Training Program

- **IGCC with CO_2 Capture**
  - IGCC Orientation for Engineers and Managers (4 days)
  - Introduction to IGCC Operations (10 days)
  - IGCC Operations for Advanced Operators (10 days)
- **Gasification**
  - Gasification Process Operations (5 days)
- **Combined Cycle**
  - Combined Cycle Operations (5 days)

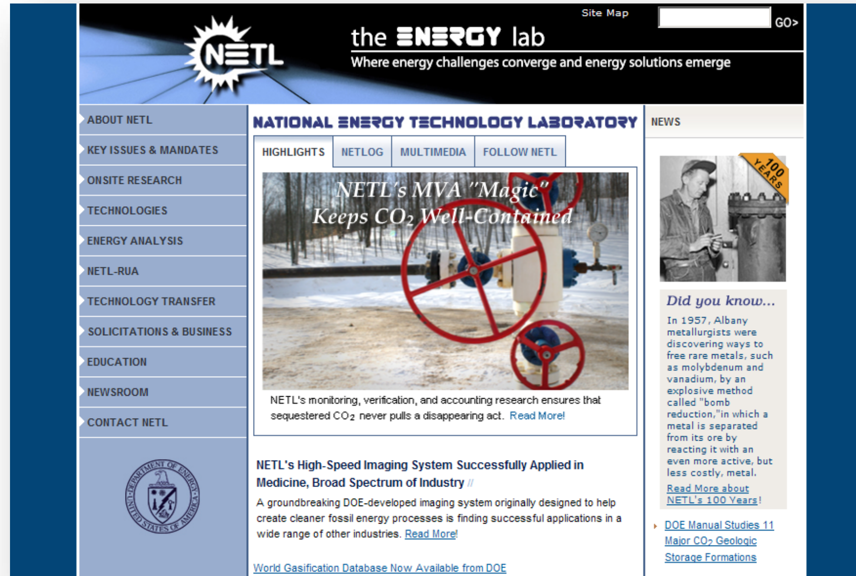




• Experienced power plant trainers • Registration inquiries and fees online • Maximum of 8 trainees per course	• CEUs through West Virginia University • Customized courses/programs available • ITS integrated into training in early 2012

For more information on AVESTAR training, please visit: www.netl.doe.gov/avestar/training.html

Questions and Additional Information



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