Overview presentation

On-Site Fuel Cell Research at NETL

October 2002

National Energy Technology Laboratory

NETL Office of Science and Technology

- **NETL Office of Science and Technology (OST)**
  – On-site research activity
  – basic and applied R&D in fossil energy and environmental science
  – 300+ DOE and Contractor personnel
  – $40 Million annual (FY01) budget - 6% of NETL budget

- **OST divided into six primary areas of research termed "Focus Areas"**
  – concentrated research topics
  – study science and technology issues facing 21st century energy production and use

NETL Focus Areas

- **Focus Areas involved in On-Site Fuel Cell Research**
  - Gas Energy Systems Dynamics (GESD)
    - Leader: George Richards
  - Computational Energy Science (CES)
    - Leader: Anthony Cugini

Gas Energy System Dynamics

Goals

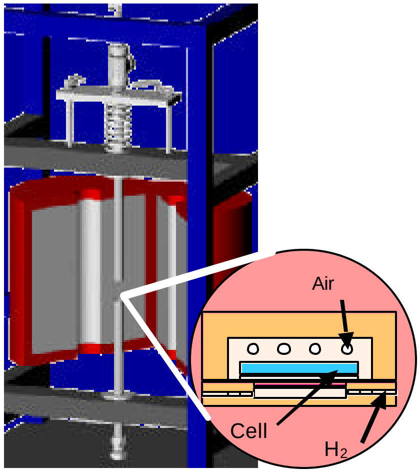
- **Develop technology to improve efficiency, “operability”, and reduce emissions in gas energy systems.**

Scope

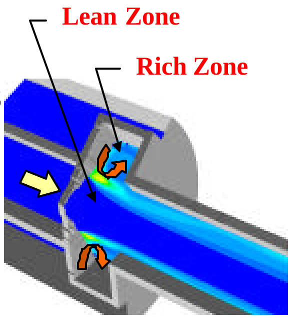
- **Power Generation from Natural Gas, Coal Gas, Hydrogen**
  - Turbines, Hybrid Turbine Fuel Cells, Reciprocating Engines
  - Fuel cells/Fuel processing for fuel cells
  - New applications (pulse, ramjet...)

Current Research Topics

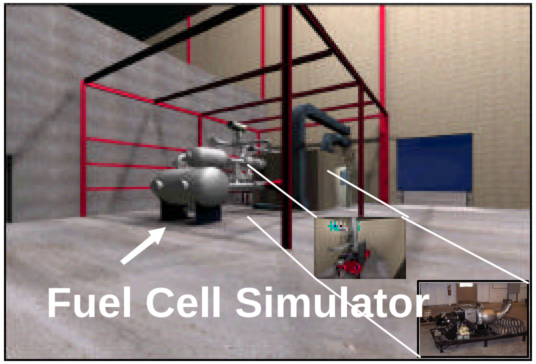
- High temperature solid oxide fuel cells
- Ultra-high efficiency from hybrid turbine/fuel cell
- Sensors and controls for *reliable* high performance
  - High temperature combustion sensors
  - MEMs distributed flow control
- Dynamics abatement in low-emission turbines
- Novel concepts including
  - “zero-emission” combustion
  - Fuel flexible turbine combustion strategies
  - Laser ignition in low-emission recips



Diagnostic measurements in operating SOFC fuel cells



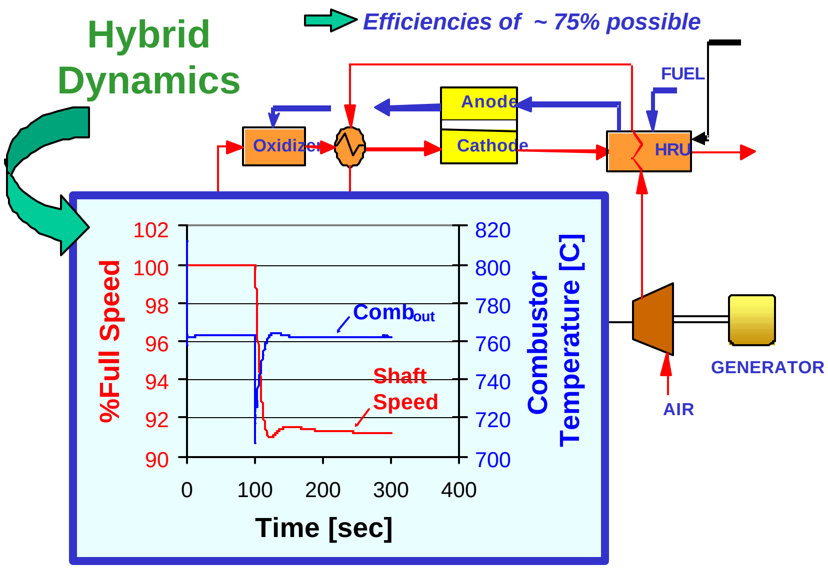
Trapped Vortex Combustor



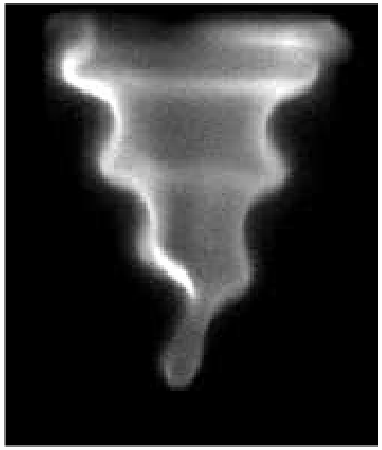
Fuel Cell/Turbine Hybrid Research Facility Design

Why Gas Energy System *Dynamics*?

- **The next generation of power generators:**
  - Complex interacting systems
  - Desire for load following
- **Opportunities and problems from *dynamic* processes.**



NETL simulation of fuel cell/turbine hybrid



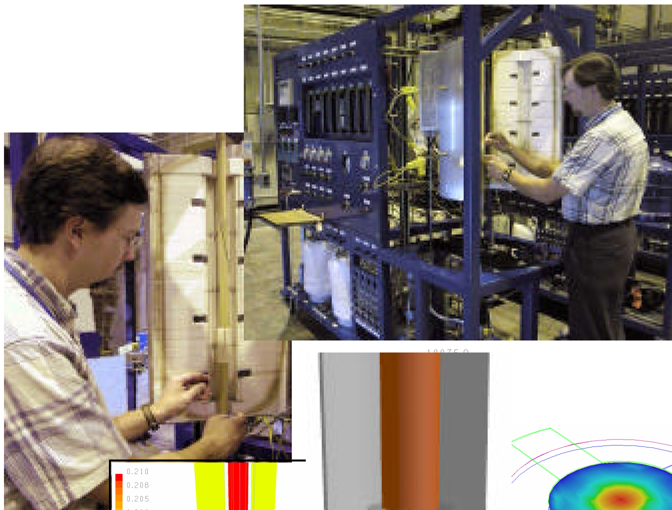
Example of flame dynamics studied at NETL

High Temperature Fuel Cell Research

Challenge: **Life, performance, cost constrained by current designs.**

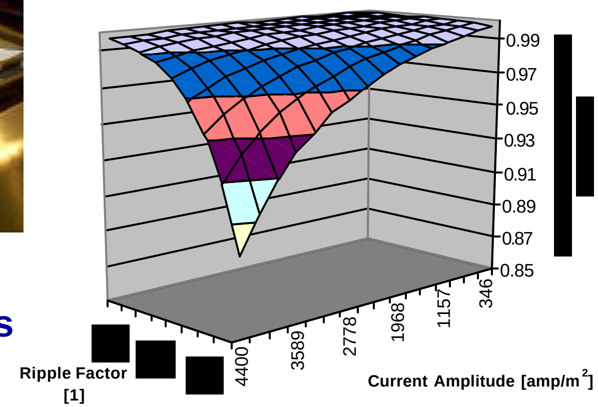
GESD research: **Identify degradation from transients, design, impurities.**

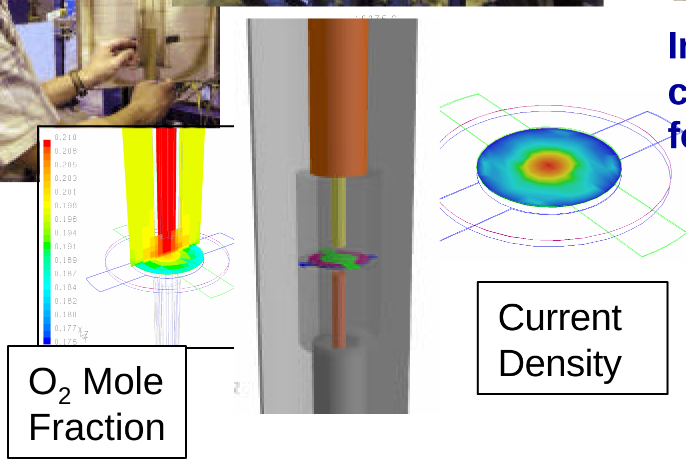
Benefit: **Validated design models, low cost components, greater impurity and transient tolerance.**



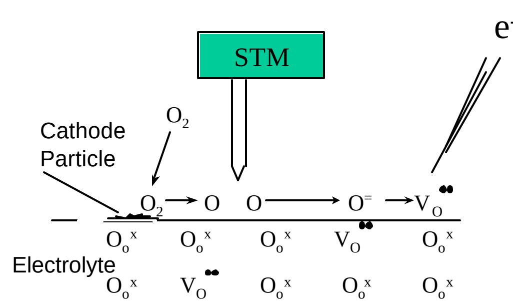
Investigation of low-cost coating technique/materials for metal interconnects

Impact of ripple current dynamics on oxygen concentrations



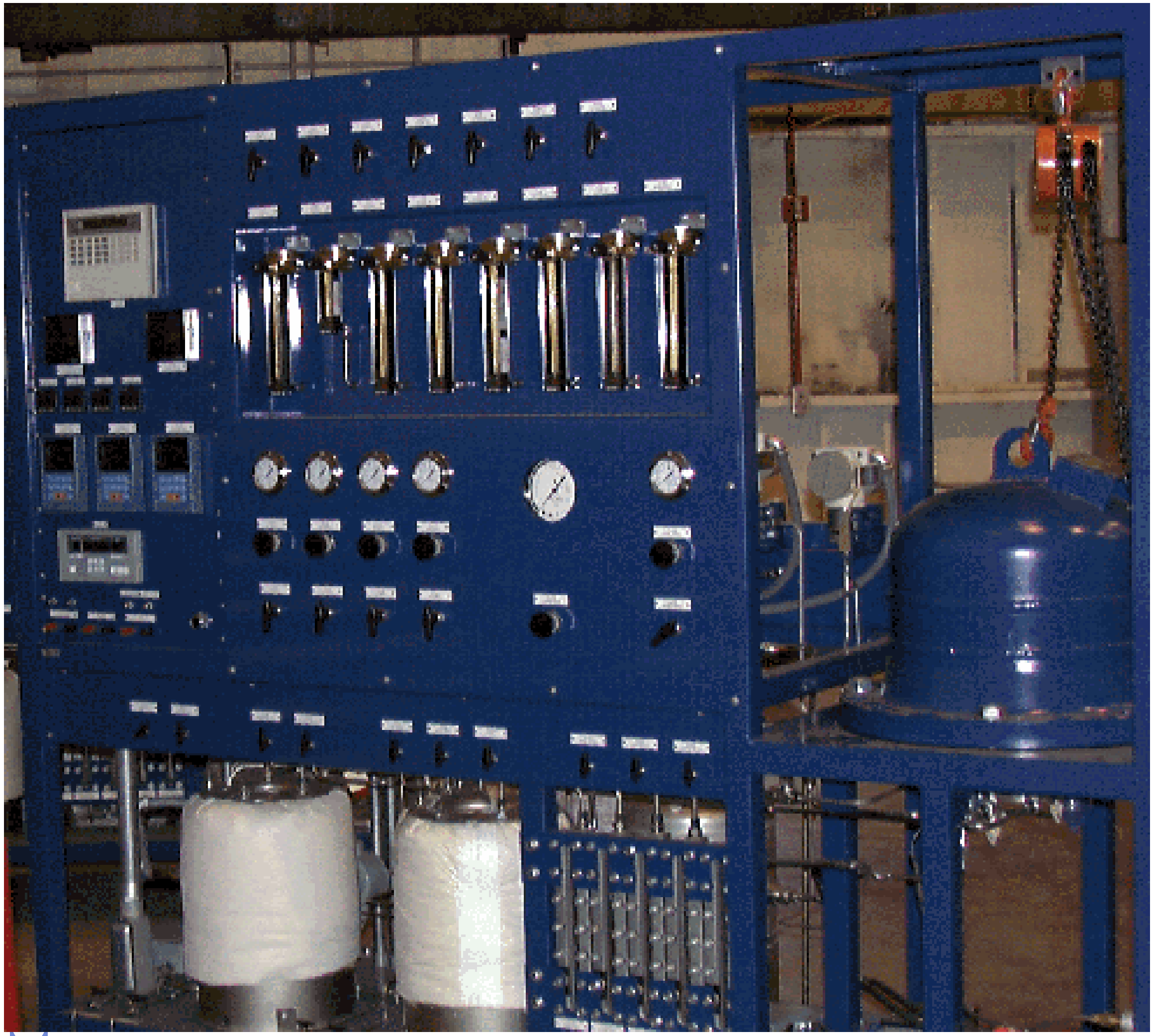


Test stands and simulations used for model validation, understanding degradation



Dynamics of oxygen at cathode/ electrolyte interface w/U Pitt & UCF Focus Area

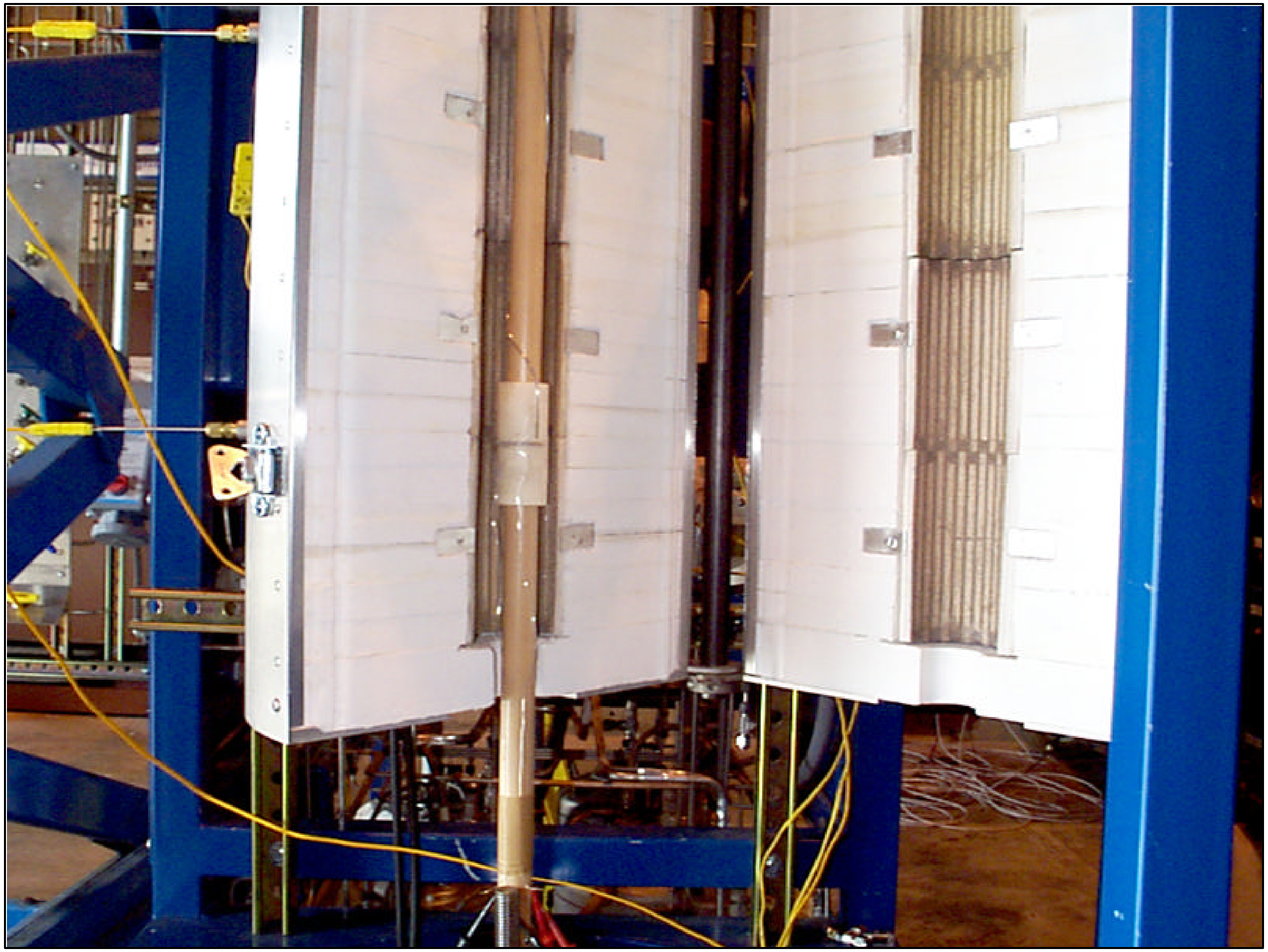
High Temperature Fuel Cell Research



NETL SOFC Test Stand

- 300 watt max
- pressure capable
- acquire test cells from partners with range of fundamental properties (component thickness, porosity, etc.)

High Temperature Fuel Cell Research



SOFC Test Stand Furnace in Button Cell Configuration

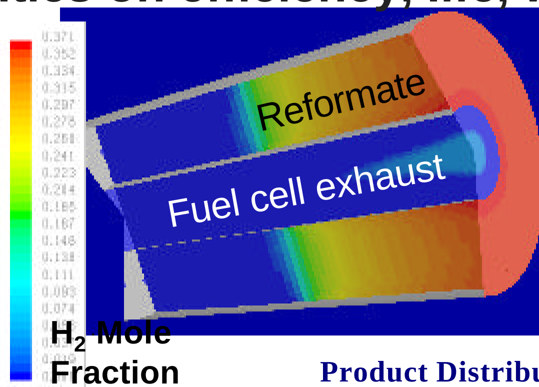
Fuel Processing for Solid Oxide Fuel Cells

Challenge: **Fuel sulfur and hydrocarbons degrade anode.**

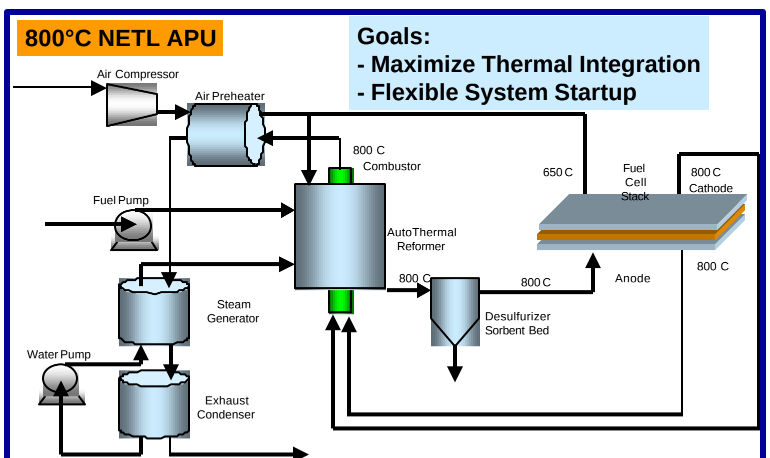
GESD research: **Desulfurization, reforming catalyst for fuel cell system.**

Benefit: **Diesel fuel use w/o penalties on efficiency, life, water requirements.**

Sulfur removal using SCOHS catalyst



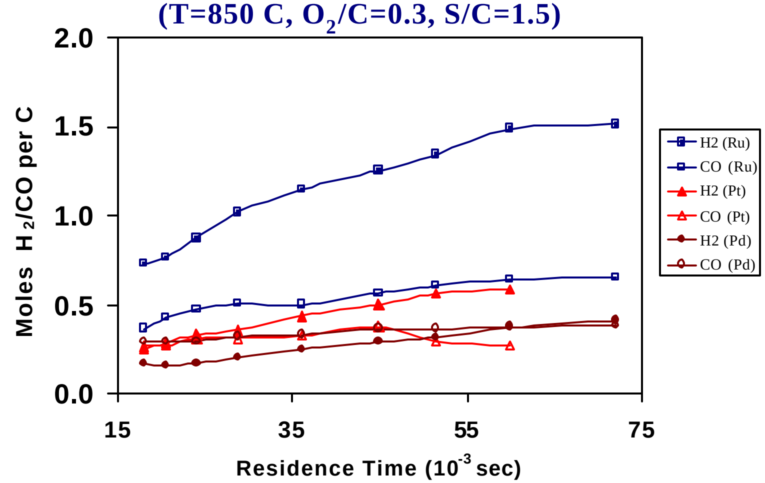
Detailed analyses of reformer integration



Fuel cell/reformer system integration studies

Product Distribution from ATR of Diesel

(T=850 C, O_2/C=0.3, S/C=1.5)



Diesel fuel reforming on various catalysts

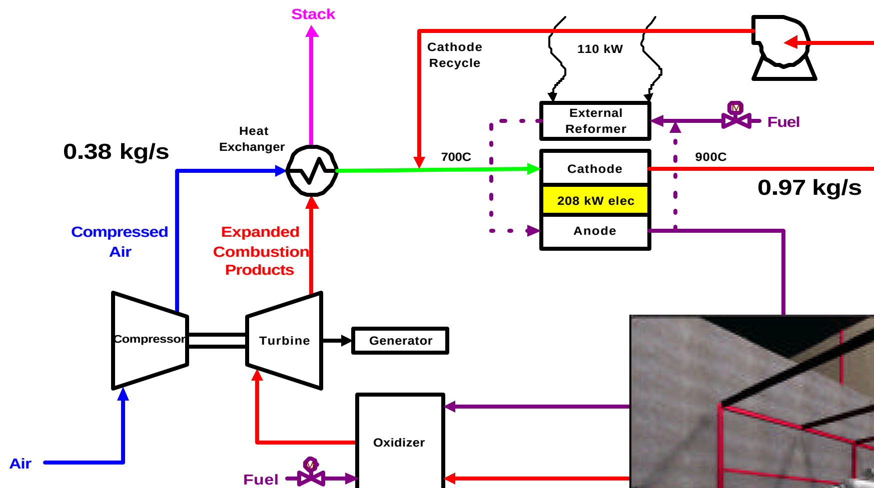
Hybrid Performance Studies (HYPER)

Challenge: **V21 efficiency goal challenged by transient handling.**

GESD research: **Model & experimental verification of system/control ideas.**

Benefit: **Public research to identify system tradeoffs for high efficiency.**

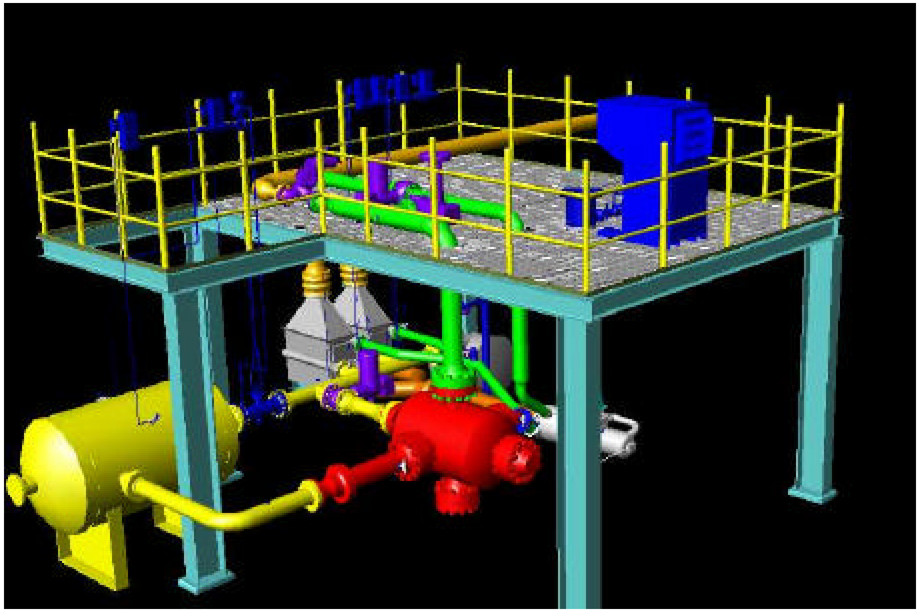
Vision 21 plants achieve high efficiency (60% coal, 70% NG) w/ hybrid turbines and fuel cells.



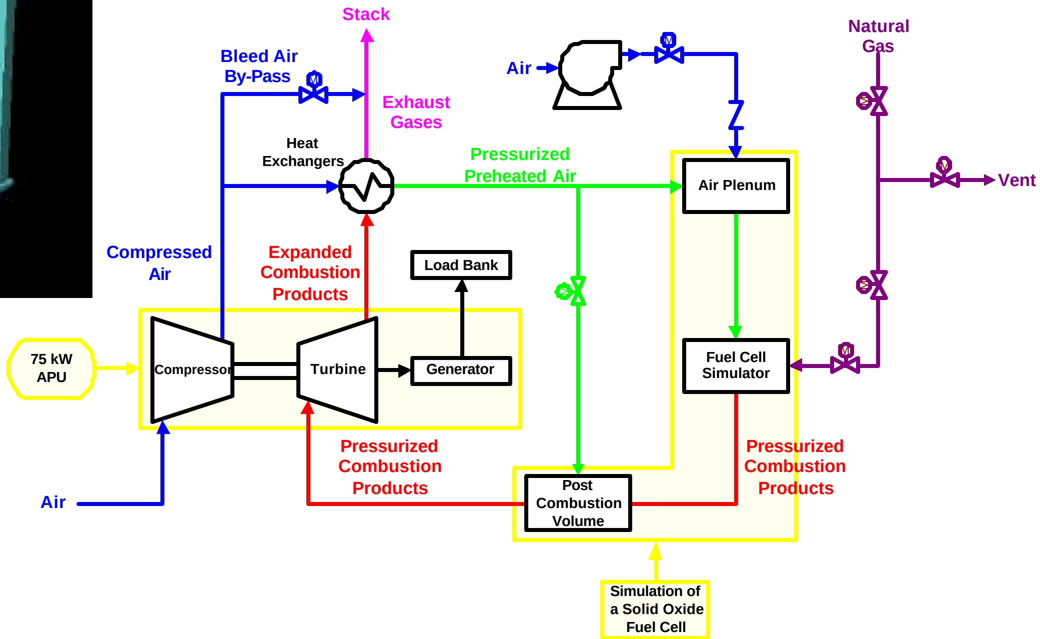
Model investigation of novel hybrid concepts: cathode recycle for thermal control

NETL Fuel Cell/Turbine Hybrid Research Facility

Hybrid Performance Studies (HYPER)



75kW APU



Sensors and Control for Power Generation

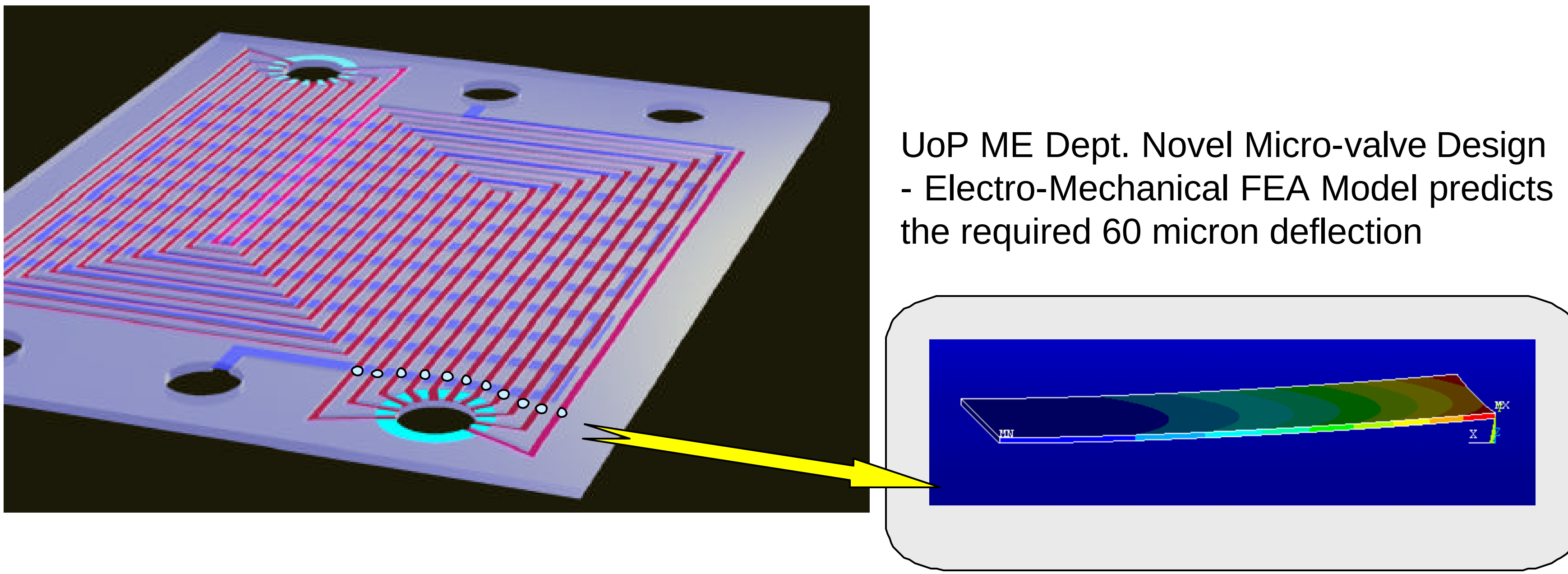
Challenge: **Advanced power systems require precise sense & control.**

GESD research: **MEM distributed flow control.**

Benefit: **Achieve improved performance, flow tolerances.**

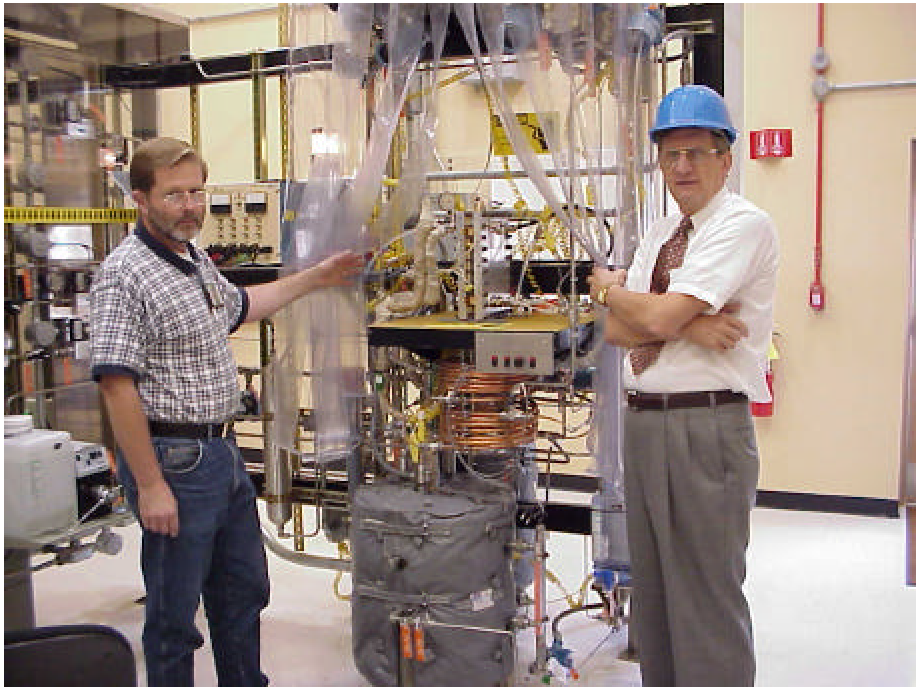
Fuel cell flow passages (red)
with MEMS valves

UoP ME Dept. Novel Micro-valve Design - Electro-Mechanical FEA Model predicts the required 60 micron deflection

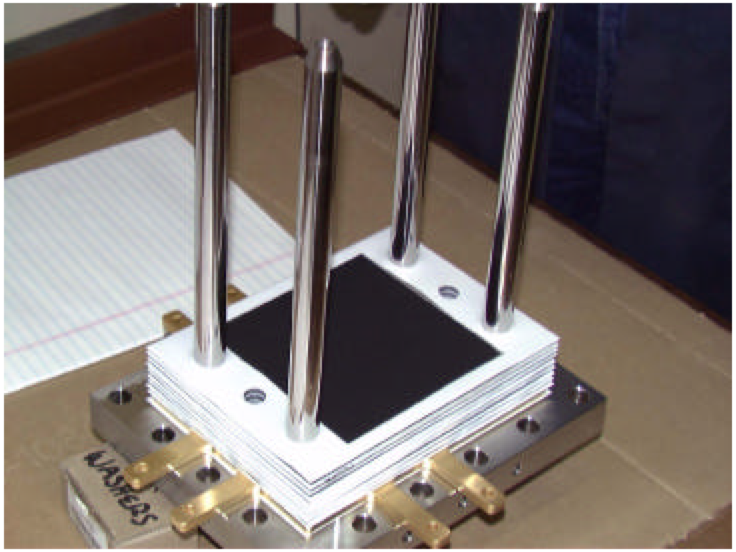


Sensors and Control for Power Generation

- **Start with PEMFC, Graduate to SOFC**
- **Experimentally confirm the benefits of cell-to-cell flow distribution in PEMFC**



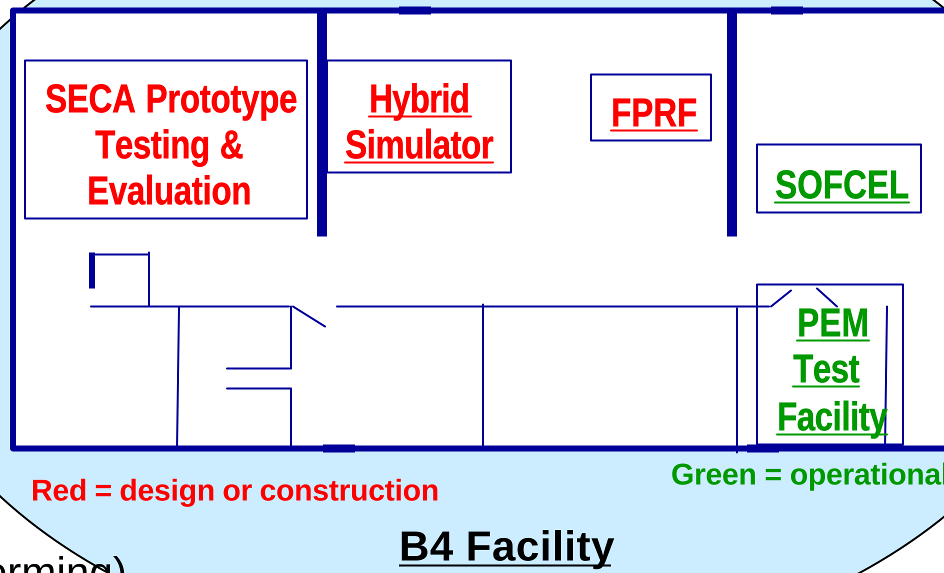
PEMFC Test Stand

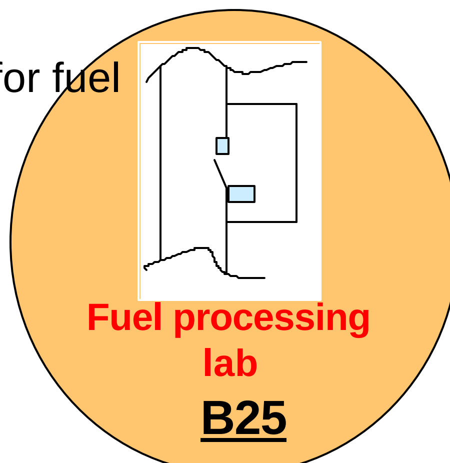


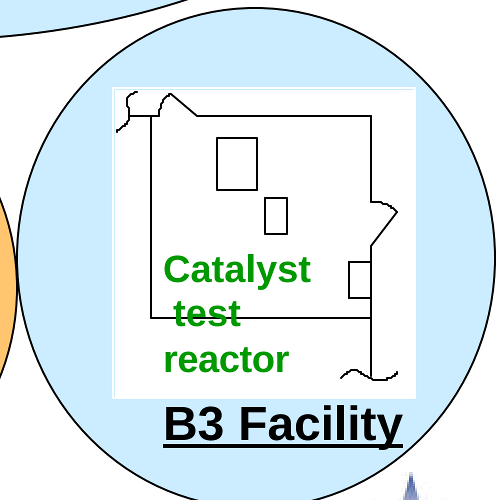
- 300 Watt (4) cell Generic PEM Stack Design
- Baseline testing conducted on generic stack for comparison data

OST Fuel Cell/Fuel Processing Facilities

- **Test Facilities:**
  - B4 (7500 sq-ft)
  - B3 (1000 sq-ft)
  - B25 (400 sq-ft)
- **Personnel**
  - 11 FTE (DOE)
  - 12 FTE (Contractor)
- **Present Capability (green)**
  - Fuel processing (clean-up and reforming)
  - Fuel cell testing (50W - 300W high temp.; 5kW low temp.)
  - Advanced sensor/controls development for fuel cells
  - Modeling (detailed and systems)
- **New capability as at right (red)**







GESD Staffing and Partnerships

- **Current research staff includes:**
  - Senior federal researchers and contractor scientists.
  - Expertise in turbine combustion, pollutant chemistry, acoustics, fuel-cell fluid flow and operation, reciprocating engines, optical diagnostics, sensors and control systems, fuel processing
- **Recent partnerships, collaborations, seminar visitors:**
  - Air Force Research Lab, Sandia, PNNL, ORNL, NASA Glenn
  - Virginia Tech, Penn State, TU Munich, Drexel, University of Pittsburgh, IIT, Georgia Tech, UT Austin, Cranfield
  - National Fuel Cell Research Center, Glennan Microsystems
  - Parker Hannifin, Solar Turbines, UTRC, GE, Fuel Cell Energy, Alzeta, Rolls-Allison, Rosemont, Woodward Controls, Siemens Westinghouse

* in discussion

Computational Energy Science

Goals

- **Develop science-based computational tools and apply them to simulate clean, highly efficient energy plants of the future**
- **Develop "virtual simulation" capability that predicts:**
  - Interactions of turbines, fuel cells, combustors, environmental control systems, and other major components
  - Dynamic responses of an entire energy plant
  - A virtual environment to visit and explore future vision-21 plants

Scope

- **Nano-Scale**
  - Computational Chemistry
- **Meso-scale**
  - Science-based constitutive laws
- **Device scale**
  - Computational Fluid Dynamics of energy conversion devices
- **System scale**
  - Coupled systems with complex interactions
  - Dynamic control
- **Visualization**
  - Computer visualization and virtual environments

CES Organization

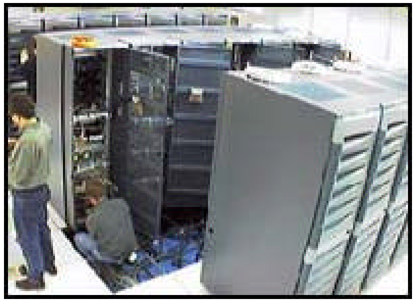
- Solids Transport Experimental Facility
- Modeling and Simulation
  - Gas-solids Flow Modeling
  - Modeling of Bubble Columns
  - Modeling of Single Phase Flows
  - Turbine Combustors
  - Fuel Cells
  - Theoretical Studies of Multiphase Flows
  - Smooth Particle Hydrodynamics
  - Black Liquour Gasification
  - Dynamic Simulations - Fuel Cells
- Supercomputing Initiative
- OIT
- Hydrates

CES Organization

- **Physical Simulation**
  - Fluidization Laboratory
- **Device Modeling / Numerical Simulation**
  - Development and validation of component models
- **Model Integration**
  - Couple models to describe a system
- **Multi-Phase Flow**
  - Challenging physics related to reacting, dense multiphase flow
- **Visualization**
  - Interpret and present model results
- **Computational Chemistry**

CES Facilities

- **Computer Hardware Resources**
  - 272 CPUs in 3 PC-Clusters, Linux OS
  - 4 terabytes of RAID storage
  - Advanced visualization laboratory
  - Multi-wall visualization environment for 3-D visualization
  - Access to Pittsburgh Supercomputer Center Resources

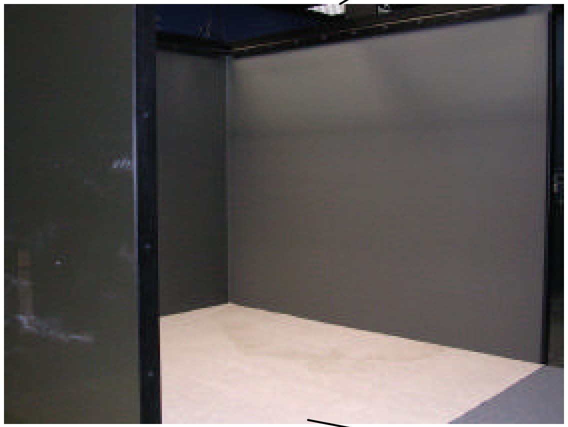


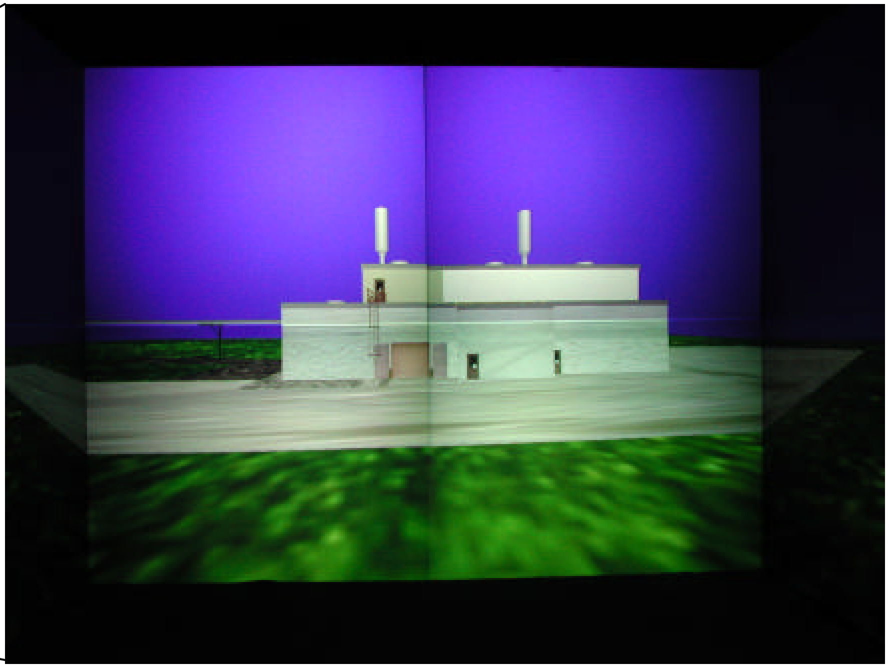
New tera-scale computer module at Pittsburgh Supercomputer Center

NETL PC-Clusters

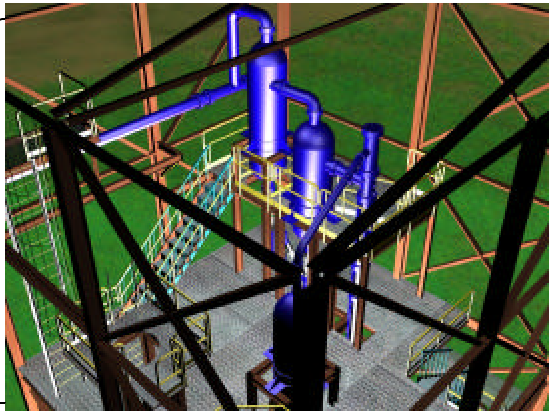
CES Facilities

- **Visualization Resources**
  - Multi-wall system





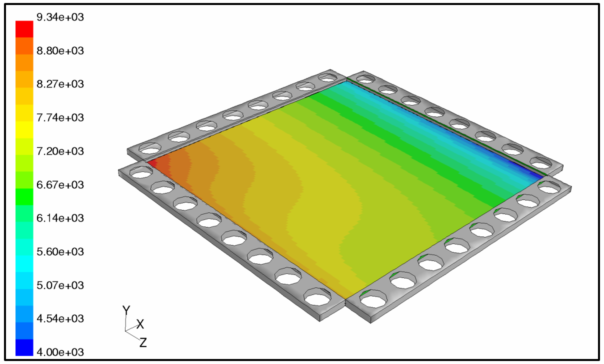
  - Visualization stations



CES Facilities

- **Computer Software Resources**
  - FLUENT license for NETL On-site use for all CPUs
  - Ensight Visualization Software
  - ANSYS FEM Software
  - Chemkin
  - AspenPLUS
  - 3D Studio Max Modeling Software
  - Virtools VR Authoring Software
  - OpenDX, Mavis, Vtk, Chromium

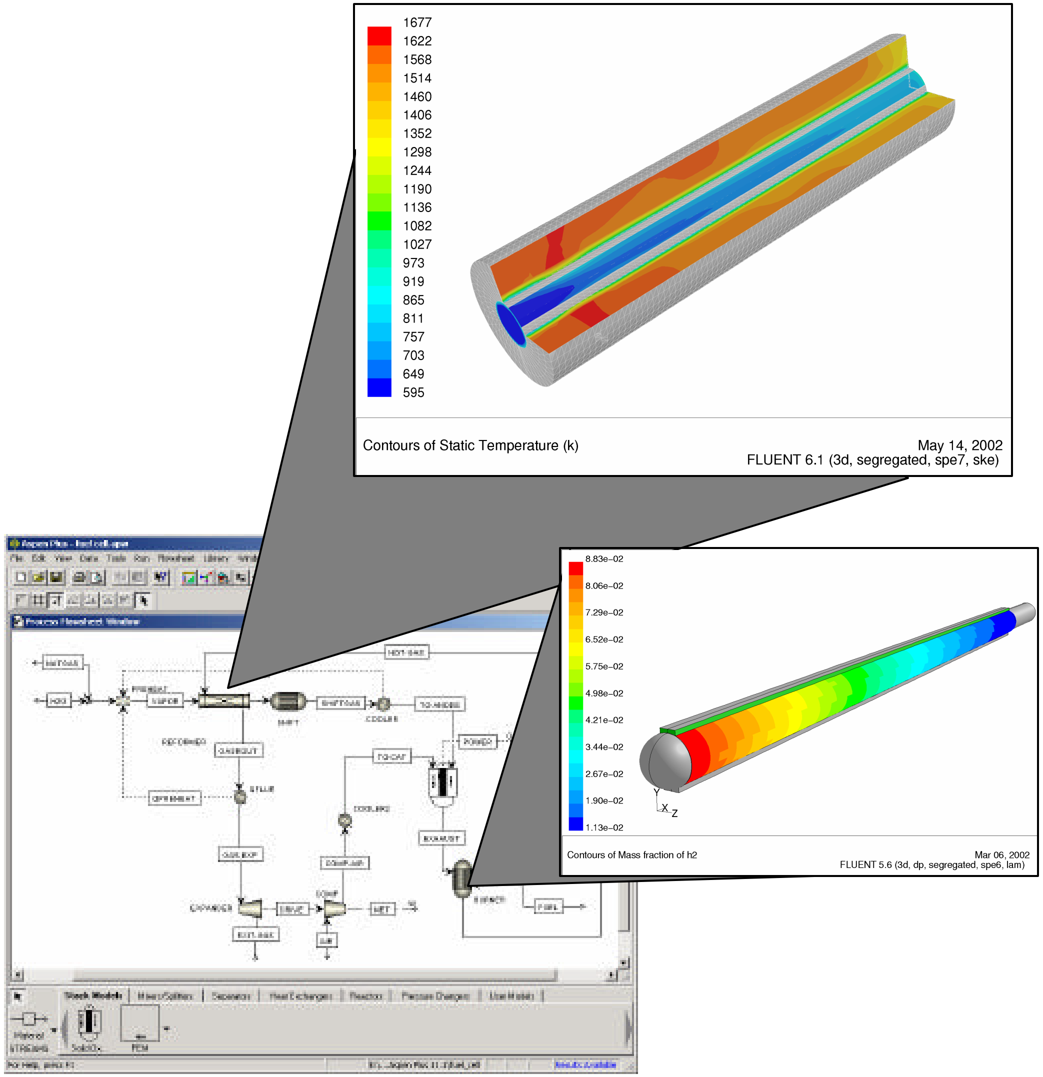
Stress in single SOFC cell at 1073K From NETL Model



Current Density on Electrolyte-Cathode Face (amp/m^2)

Developing Capabilities

- Development under Vision 21 program
- Example of fuel cell power system process modeled with Aspen Plus
- 3-D reformer model and SOFC models based on FLUENT CFD are integrated with the flow sheet model
- Inflow stream data, physical properties and reaction kinetics data are transferred from Aspen Plus to FLUENT
- Outflow stream data are transferred from FLUENT to Aspen Plus



Software Architecture