1) SECA Phase I Validation Testing
2) Coal Gas Impurity Studies

2007 SECA Workshop

August 7-9, 2007

Dr. Randall Gemmen

Energy Systems Dynamics Division

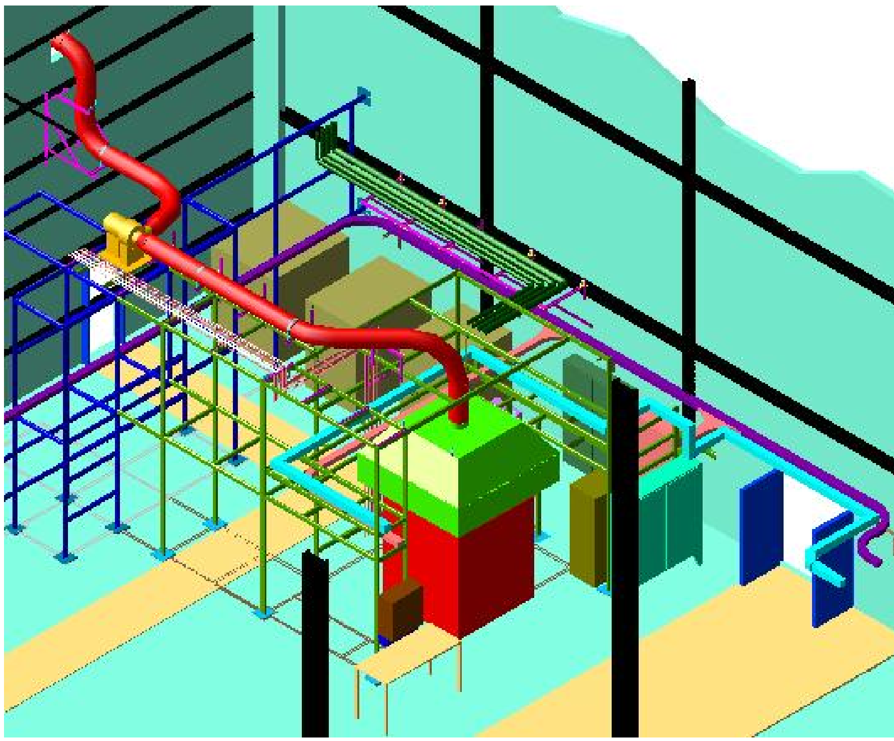
National Energy Technology Laboratory

Projects for Review Today

- **1) DOE Fuel Cell Test Facility**
  - Independent Testing for SECA Program

- **2) Coal Contaminant Investigations**
  - Focused Studies Using Specific Contaminants
  - Direct Coal Syngas Studies

1) DOE Fuel Cell Test Facility



Objectives

Support DOE's SECA Program by providing independent test and evaluation of its sponsored partner's SOFC fuel cell systems (each done <u>separately</u>)

Challenges

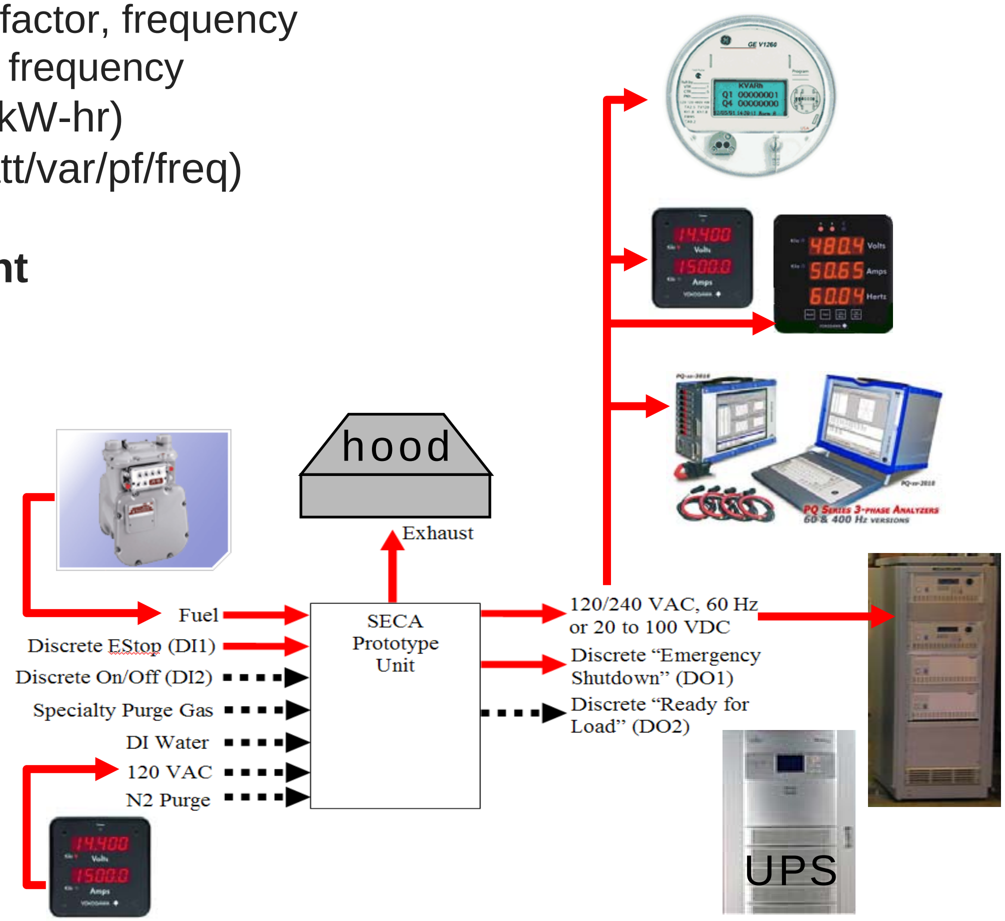
Accurately measuring the critical performance parameters

Approach

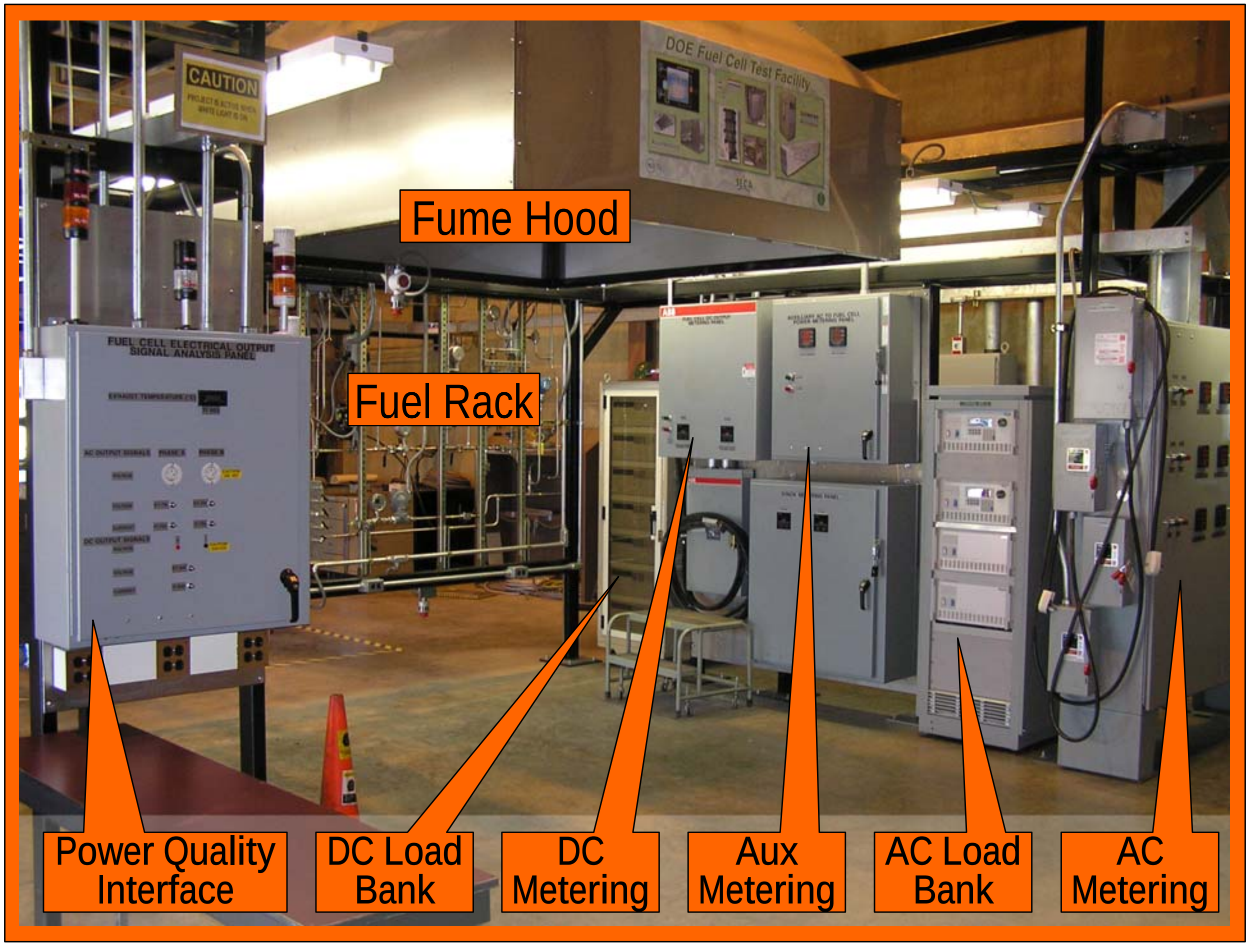
- ☑ **Define test facility requirements based on SECA Industry Team SOFC unit specifications**
- ☑ **Apply relevant industry test standards**
  - – PTC 50-2002
    - Performance analysis standards
    - Error analysis standards
- ☑ **Base-Design by Concurrent Technologies Company**
- ☑ **Phased construction through 2010**
  - ☑Natural Gas/Methane (2006)
  - ❑Synthesis Gas for Coal-Based FC (ca. 2008-20010)
- ☑ **Measurement Methodology**
  - – Gemmen & Johnson (2006), "Evaluation of Fuel Cell System Efficiency and Degradation at Development and During Commercialization" J. Power Sources.
- ☑ **SECA prototype evaluations**
  - – Shake-down testing (Acumentrics unit)
  - – Evaluate prototype systems
  - – Report results to SECA management

Instrumentation

- **0-12kW AC and DC load banks and load profile controller**
- **Continuous power measurement**
  - Aux Input: real power, power factor, frequency
  - AC: real power, power factor, frequency
    - Revenue quality meter (kW-hr)
    - Solid state metering (watt/var/pf/freq)
  - DC: power
- **Continuous fuel measurement**
  - High accuracy corriolis meter
  - On-line GC for fuel energy
  - Revenue quality meter
- **Safety instrumentation**
- **Safety communication**
- **Exhaust gas analysis**
- **On-line UPS system**
- **Vent hood**
- **Purge gas**
- **DI-water**
- **Spare I/O capability**



DOE Fuel Cell Test Facility



Control Room

Procedure

- Begin close coordination with fuel cell developer
- Communicate all detailed test unit requirements and facility capability/limitations
- Account for critical safety requirements on both sides
- Perform engineering documentation updates and facility modifications
- Install test unit
- Perform all critical equipment calibrations
- Startup test unit, and perform operational checkout
- Initiate test plan
- Complete test plan and shutdown test unit
- Perform post-calibrations on all critical equipment
- Analyze and report test results to SECA Mgmt.

Units Tested

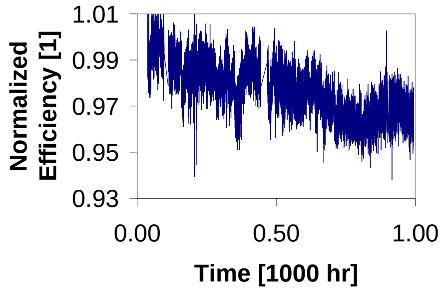
- overall efficiency > 35% stationary
- degradation <2%/500 hr
- peak power

FCE/VPS

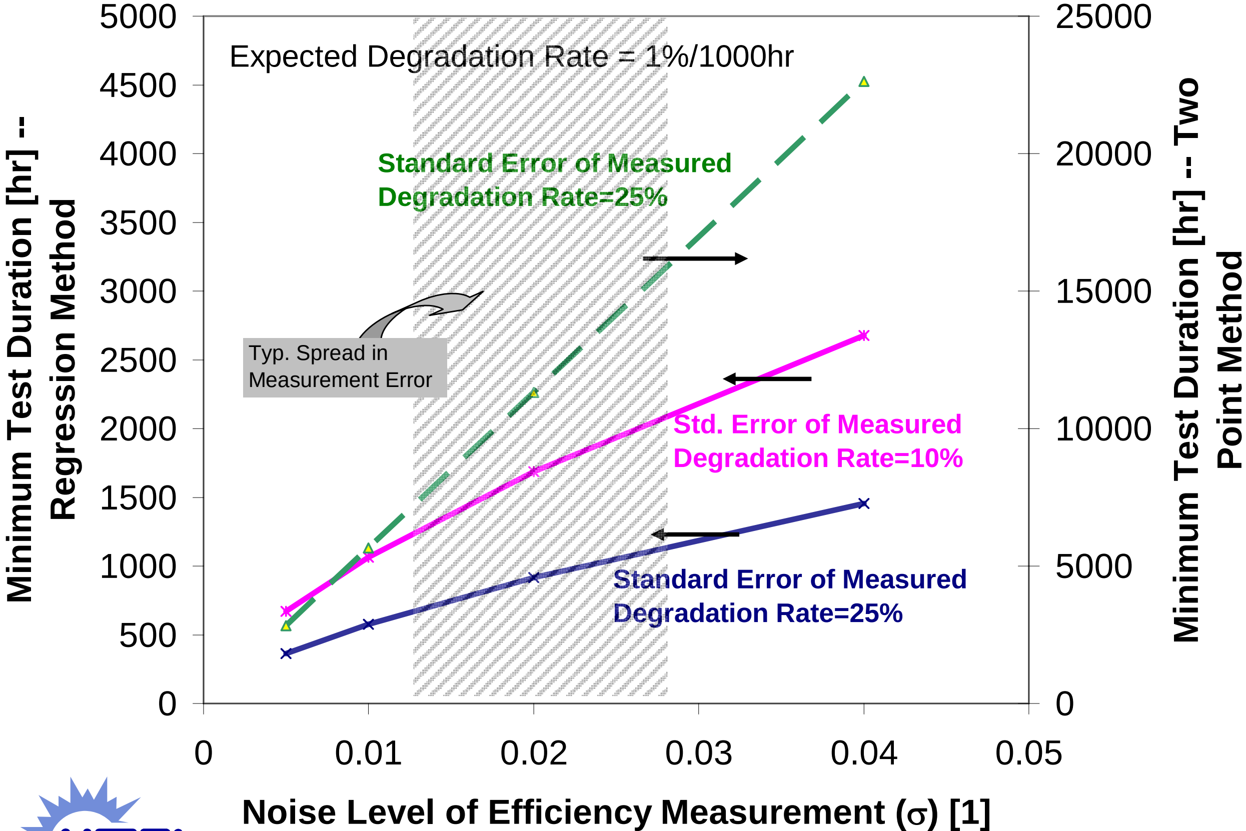
Delphi

Acumentrics

Degradation Measurement



What length of time must test run to assess the degradation rate to within a certain X% accuracy?



From 2-Point (end-start):

$$SV = 2 \cdot \sigma^2$$

From Regression:

$$SV = \frac{\sigma^2}{\sum_{i=1}^{N} (t_i)^2 - \frac{\left(\sum_{i=1}^{N} t_i\right)^2}{N}}$$

SV = variance of the measured slope (degradation).
σ = standard error of measurement value.
t_i = time value for data point ‘i’.

2K-2571

Results

Summary

- **Government programs need to measure progress in meeting goals…SECA has accomplished this through independent test and evaluation of developer technology**
  - Three SECA units tested
  - Results show performance meeting SECA Program objectives

- **Future:**
  - Transform facility to support evolving SECA Coal-based Program.

NETL

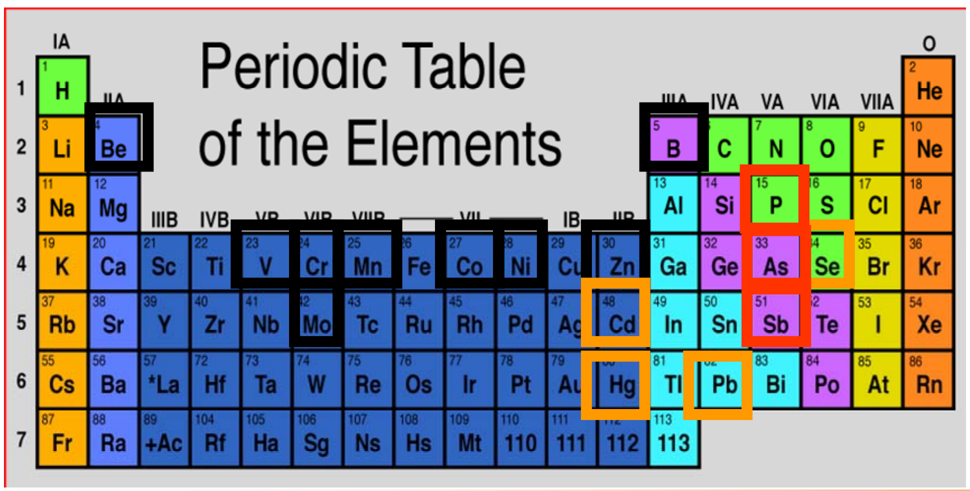
2K-2571

2) Coal Contaminant Investigations

Kirk Gerdes, Jason Trembly, Randall Gemmen

Objectives

- **Objectives**
  - Determine the effect of trace coal syngas species on the performance of solid oxide fuel cells
- **Challenges**
  - Little research has been completed investigating behavior of SOFCs operating on coal syngas
  - Many possible interactions between trace species contained in coal and SOFC materials
  - Coal contains many trace species so a very large effort will be required to screen the affect of all of the contaminants



•present in coal syngas

•present in coal syngas;
•not removed by warm-gas cleanup

•present in coal syngas;
•not removed by warm-gas cleanup;
•potential reaction with anode

Approach

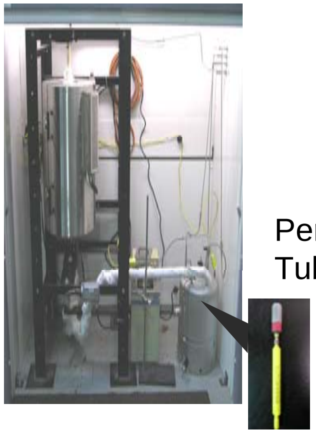
- Thermodynamic studies
  - **Warm/hot gas cleanup system/trace specie interactions**
  - **Gaseous trace specie/SOFC anode interactions**
- Electrode transport modeling
  - **Dust Gas Model (DGM)**
  - **Mean Transport Pore Model (MTPM)**
- Experimental study of individual trace species on SOFC performance
  - **HCl, H_2S, AsH_3, PH_3, H_2Se**
  - Syngas (Kivisaari et al.): 29.3%H_2, 28.7% CO, 11.8% CO_2, 27.2% H_2O, 3% N_2
- Experimental study on direct coal syngas

Effect of Trace Species on SOFC Anode

- **Affect the ability of Ni to promote the electrochemical reactions**
  - Trace species on Ni surface inhibit the adsorption of H_2, CO, or dissociation of H_2
- **Affect the ability of YSZ to transport oxygen ion**
  - Formation of secondary zirconia phases
- **Affect the electrical conductivity**
  - Formation of secondary nickel phases such as nickel-phosphide

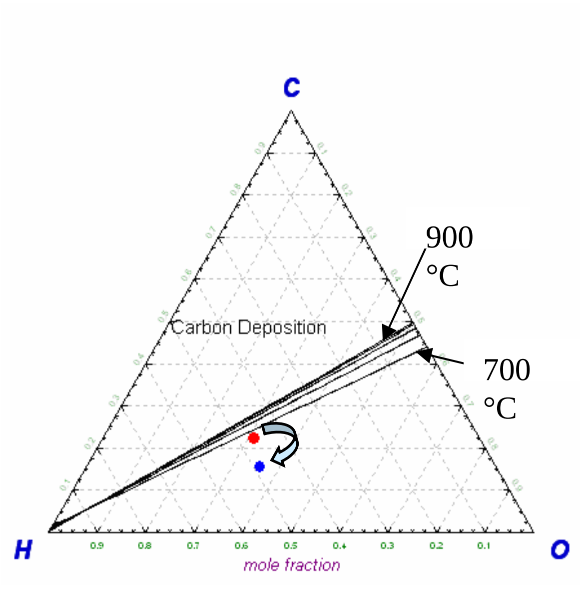
Experimental Methodology

- Anode supported SOFCs with Ni/YSZ anodes operated between 750-800ºC
- Cells operated with simulated coal syngas containing single trace specie of interest
- VI scans and EIS methods used during testing
- Post trial SEM, EDS, and XRD used



Permeation Tube

Ca—Pt Mesh/Paste;
An—Ni Mesh/Paste



Warm Gas Cleanup

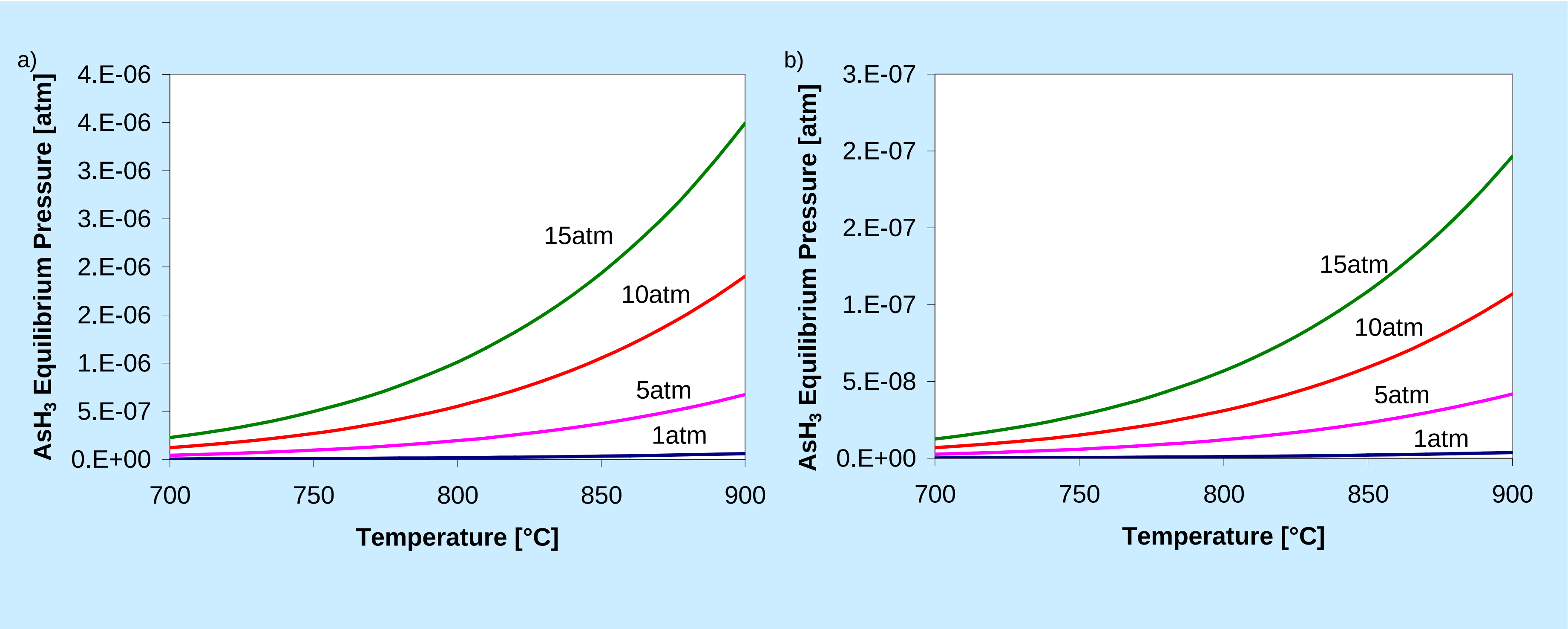
(Thermodynamic Predictions—FactSage. v. 5.4)

Component	Behavior	Concentration After Cleanup ppmv
As	**Gas/Solid**	**0.6**
P	**Gas/Solid**	**1.91**
Sb	**Gas**	**0.07**
Cd	**Gas/Solid**	**0.011**
Be	Solid	
Cr	Solid	
Hg	**Gas**	**0.025**
K	Solid	
Se	**Gas/Solid**	**0.15**
Na	Solid	
V	Solid	
Pb	**Gas/Solid**	**0.26**
Zn	Solid	

Anode Interactions

(Thermodynamic Predictions—FactSage v. 5.4)

$$AsH_3(g) + Ni(s) \rightarrow NiAs(s) + 1.5H_2(g) \qquad \text{Eq.1}$$



Equilibrium Pressures of AsH_3 Associated with Equation 1 Over SOFC Operation Conditions at the Inlet (a) and Outlet (b).

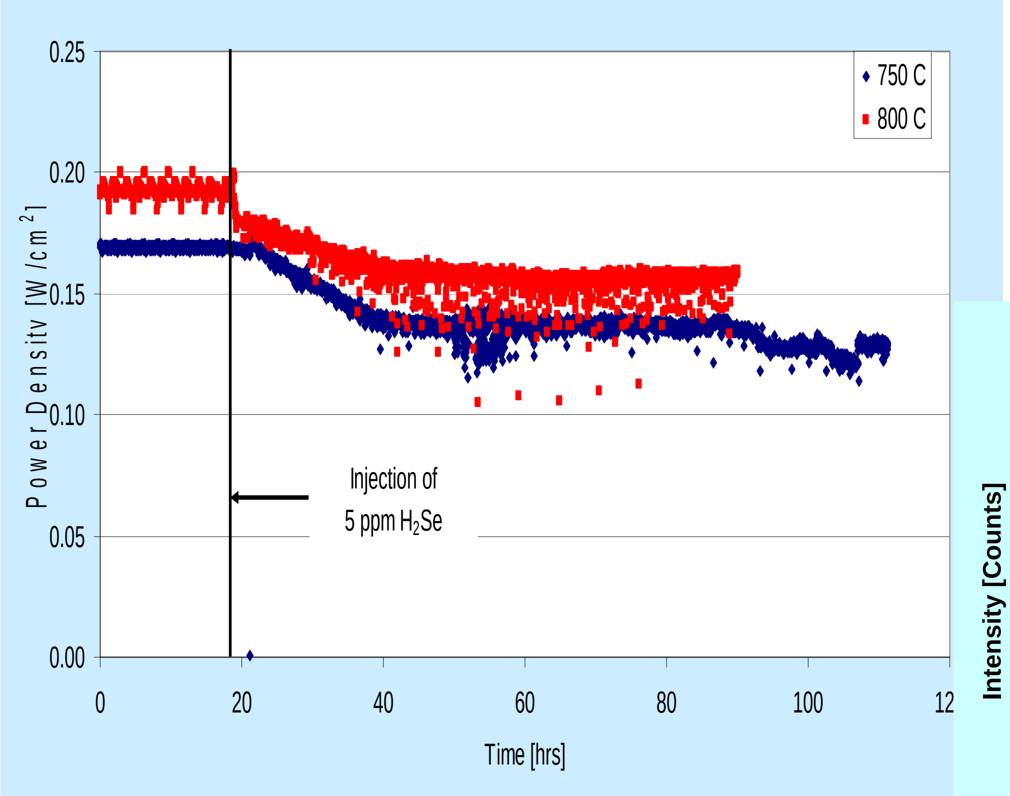
NETL

Summary of Anode Interactions

(Thermodynamic Predictions)

- **Species passing through warm gas cleanup:**
  - Sb, As, Cd, Pb, Hg, P, Se
- **At the maximum level of trace specie concentration entering the anode, the potentially anode reactive species are:**
  - Sb, As, P
- **(Other species may still impact cell performance through reaction at the surface; e.g., S.)**

Results: H_2Se Testing



thermodynamic calcs. show no tendency toward forming secondary Ni phase

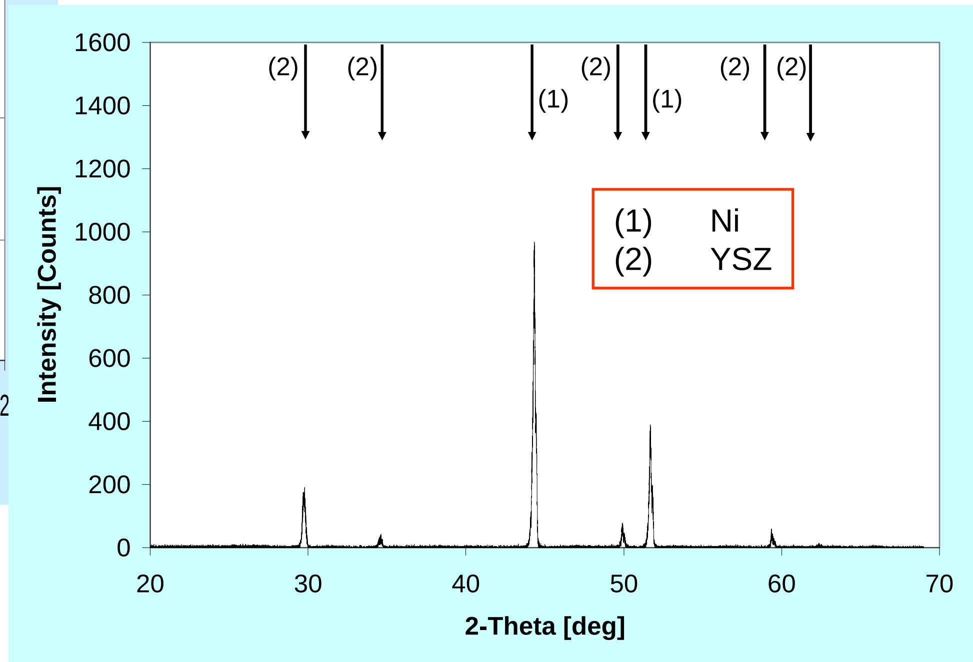
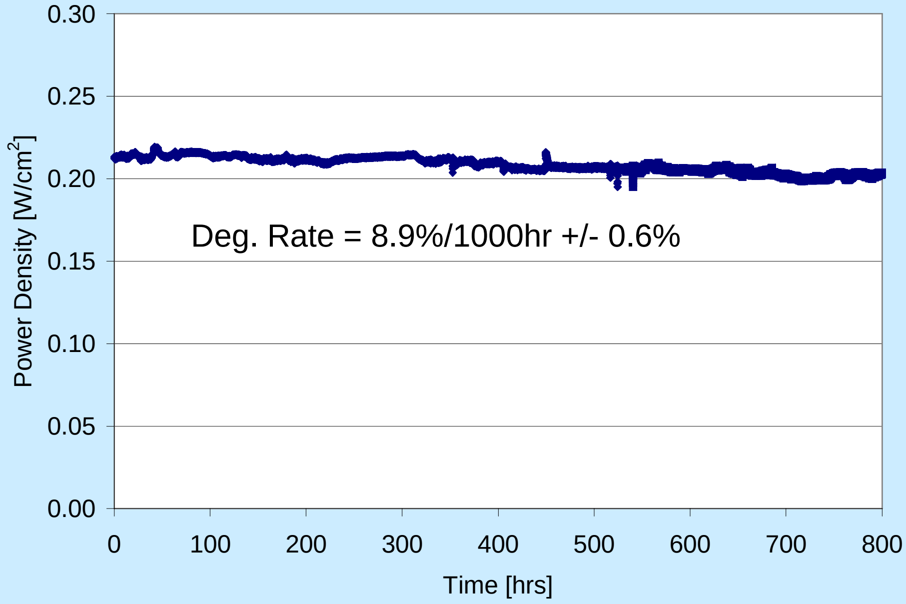


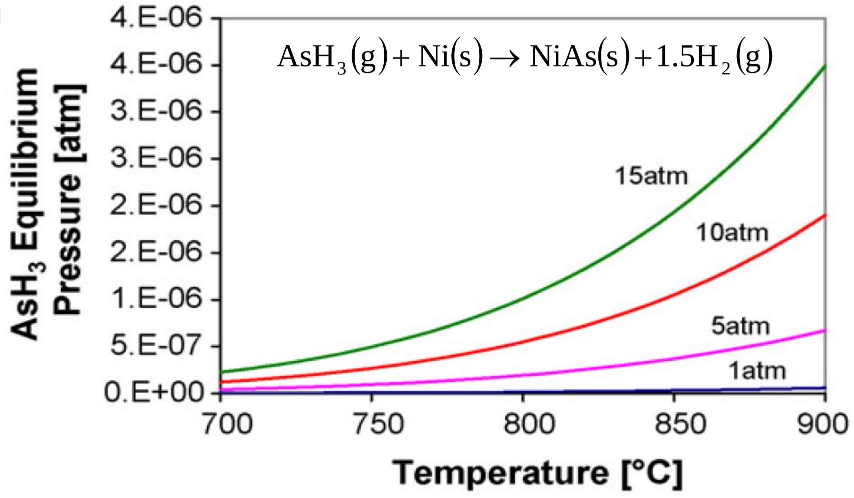
Figure 5. SOFC Power Density Operating at 750 and 800 °C at 0.25 Acm^{-2} Over Time with 5 ppm H_2Se.

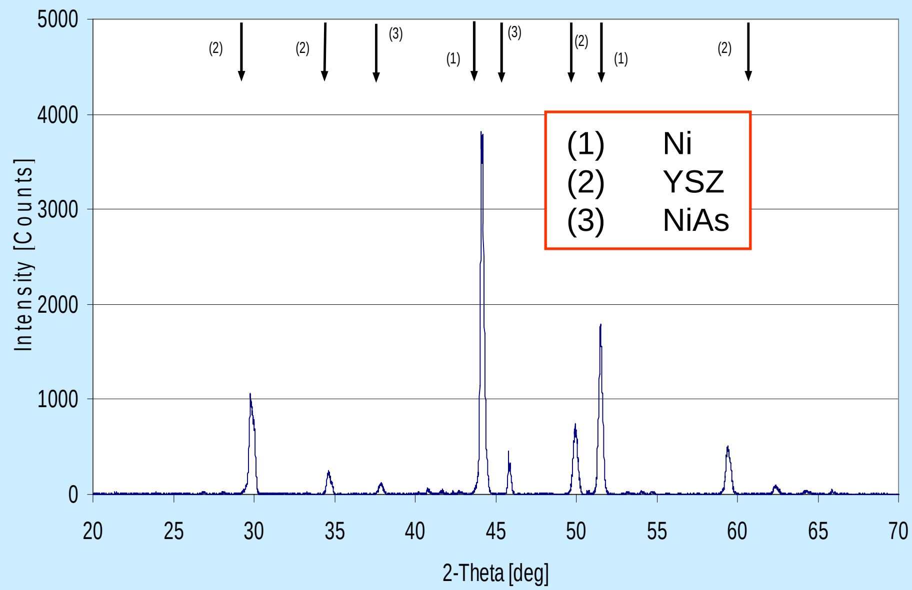
NETL

2K-2571

Results: Arsine Testing



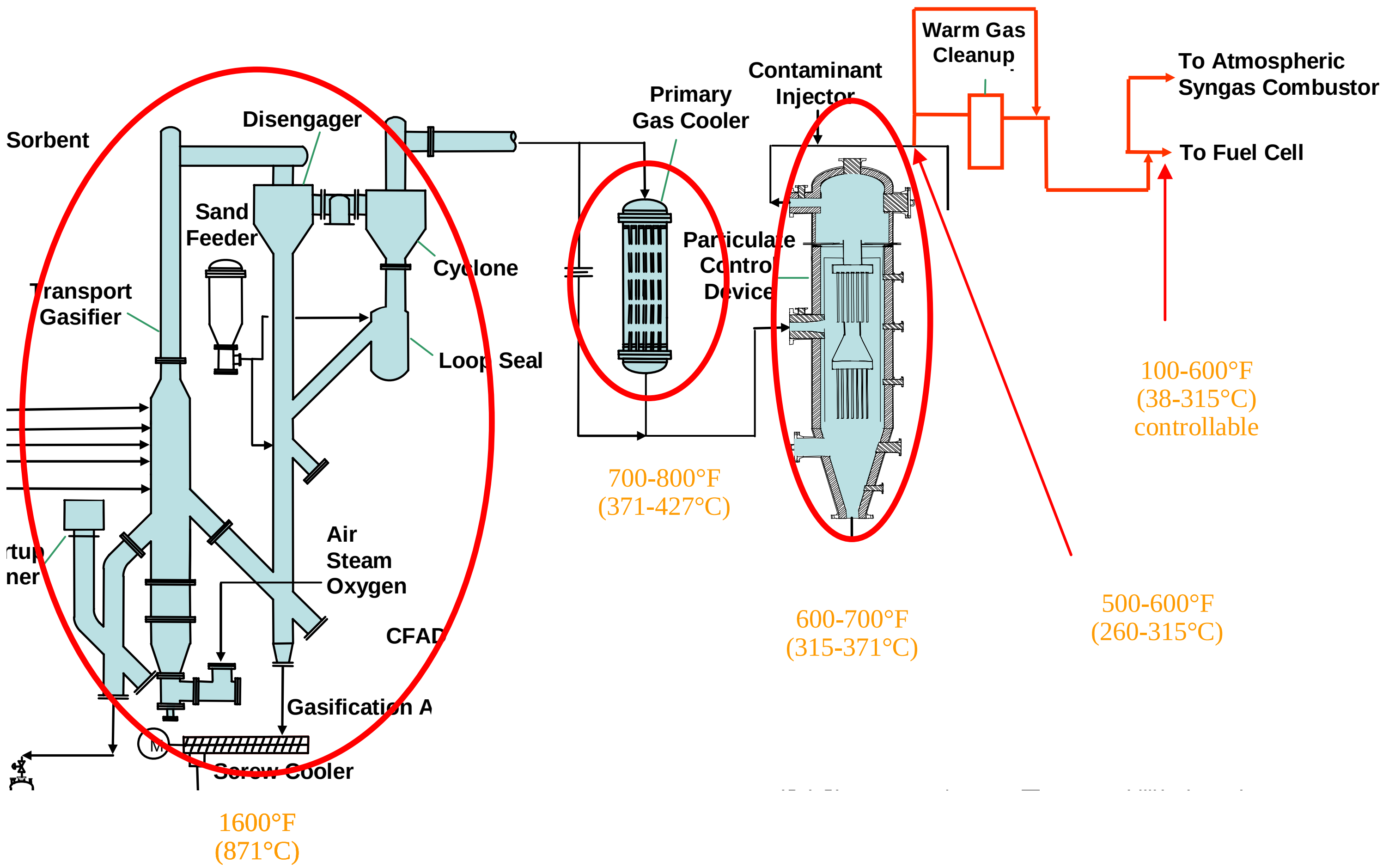




SOFC Power Density and XRD Spectra Operating at 800 °C and 0.25 Acm^{-2} Over Time with AsH_3 Concentration of 0.1 ppm.

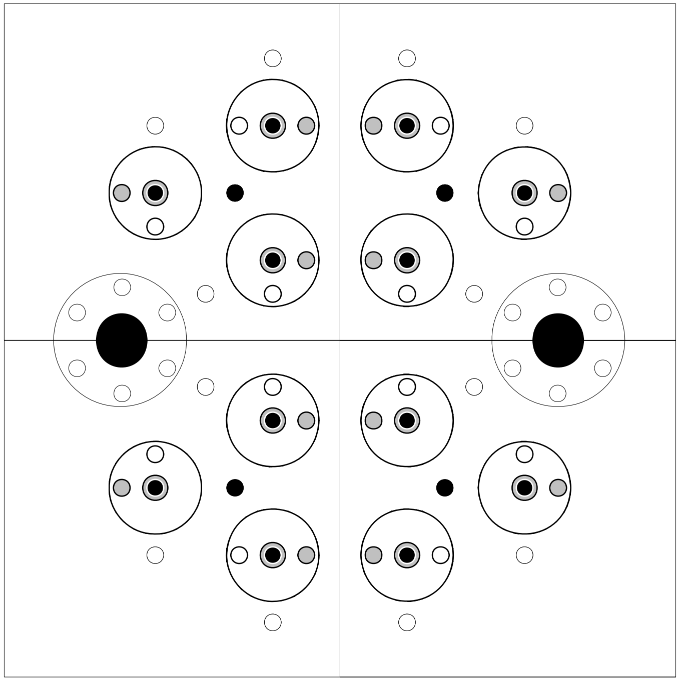
SOFC Operation on Direct Syngas

PSDF Process Flow Diagram



Test Rig
Multi-cell Array

- **Permits parallel operation of 12 button cells**
- **Divided into 4 channels of 3 cells each**
- **Improves testing method**
  - Rapid collection of repeat data
  - Reduces systematic experimental error
- **Reduces sources of contamination**
  - Seals
  - Materials



- **Status**
  - Final design completed
  - Rig construction underway
  - Shakedown testing by Oct.
  - Field testing in Jan., 2008

NETL

Summary

Contributions to program

- Performance of SECA Phase I units validated
- Effect of trace species on SOFC performance being quantitatively assessed via focused specie evaluation and direct syngas testing
- Obtaining improved measurements of gas phase contaminant concentrations (GC/ICP/MS) in coal gasification derived syngas
- Development of MCA accelerates all SOFC testing, particularly in materials and components areas