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DOE Hydrogen Program

Hydrogen Quality Issues for Fuel Cell Vehicles

DOE Hydrogen Quality Working Group: Activities and Progress

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Overview

Timeline

- Project start date: FY 2006
- Project end date: Open
- Percent complete: N/A

Barriers

- B. Stove-Piped/Siloed Analytical Capability
  - Segmented resources
- D. Suite of Models and Tools
  - Macro-system models

Budget

- Funding, FY 07: $435 K
- Funding, FY 08: $800 K

Partners/Collaborators

- OEMs, Energy Companies, National Laboratories
- Project management: Argonne

Objectives

- Assess how fuel quality influences the life-cycle costs and performance of the overall “hydrogen system” – production, purification, use in fuel cell vehicles, and analysis and quality verification
  - develop models to evaluate the quantitative effects of fuel quality on the costs of the hydrogen system components

- Identify information gaps and the R&D needed to fill those gaps

- Develop a roadmap that determines the significant cost elements, identifies challenges to reducing those costs, and makes recommendations on how to address those challenges

Milestones

Month-Year	Milestone
Nov-07	Identify one or more R&D areas to fill a gap in critical information *Hydrogen sampling and analysis for quality verification identified as a major challenge (technology, cost)*
Dec-07	Establish hydrogen purification cost versus contaminant level for four contaminant species *SMR-PSA model has been developed and preliminary results discussed in several forums*
Aug-08	Develop quantitative models for lifecycle costs of fuel cell vehicles (including the cost of H_2) versus contaminant level for four contaminant species *Results of impurity effects modeling of fuel cell performance will be used to assess effects on fuel cell costs*

Approach

- Convene a DOE Hydrogen Quality Working Group comprised of
  - representatives of various Tech Teams
  - automobile OEMs and fuel cell developers
  - energy companies
  - national laboratories
- Focus on the various significant issues
  - obtain input from fuel cell developers, gas suppliers, etc.
  - obtain input on gas analysis technologies, corresponding ASTM activities, costing methodologies
- Initiate a database of critically assessed relevant published literature
- Determine influence of varying the desired fuel quality on cost of H_2 production / purification
- Work with model developers at Argonne and other organizations to help develop and validate performance and life-cycle cost models
- Determine what R&D and/or data are needed to effectively address the issues identified

Major recommendations in the draft H2QWG Roadmap

- Hydrogen production / purification
  - determine ranges of concentrations of N_2, CH_4, CO, and other species as a function of production process design and operating conditions
  - develop quantitative models for the PSA process
  - analyze trade-offs in H_2 quality, H_2 recovery, and production efficiency
- Use of H_2 in fuel cells (if appropriate models can be developed and validated)
  - evaluate design and operating parameters (e.g., electrocatalyst loading, purge rates) to enable operation on various levels of contaminants
  - correlate design parameters with lifecycle costs of fuel cell systems
- Hydrogen analysis and quality verification
  - develop and validate (e.g., ASTM certified) analytical techniques to sample, monitor, and analyze dispensed H_2
  - develop standardized methods (even if expensive) to calibrate simpler/ less expensive methods and instrumentation for field use

Summary of activities since May 2007

- Conducted a fuel quality modeling workshop at Argonne (with Jim Ohi) to discuss PSA and fuel cell impurity effects modeling (Aug-07)
- Participated in ISO WG12 meetings and held in-depth discussions on modeling impurity effects on fuel cell systems (Nov-07, Apr-08)
- Presented and discussed H2QWG work at several FreedomCAR and Fuel Partnership's Technical Team meetings and at other forums (May-07, Jun-07, Oct-07, Nov-07, Jan-08, Apr-08)
- Developed PSA performance models for different design and operating conditions and levels of various contaminants in product H_2
- Developed methodology to evaluate cost effects using H2A

Developing the SMR-PSA performance model

- Plant Size : 1,500 kg/day of H_2 leaving the PSA unit
- Steam-Methane-Reforming (SMR) + Water-Gas-Shift (WGS)
  - Steam / Carbon Molar Ratio : 3 – 6
  - Pressure : 8-22 atm
  - Gases exit SMR at equilibrium at 750°C
  - Gases exit WGS at equilibrium at 435°C

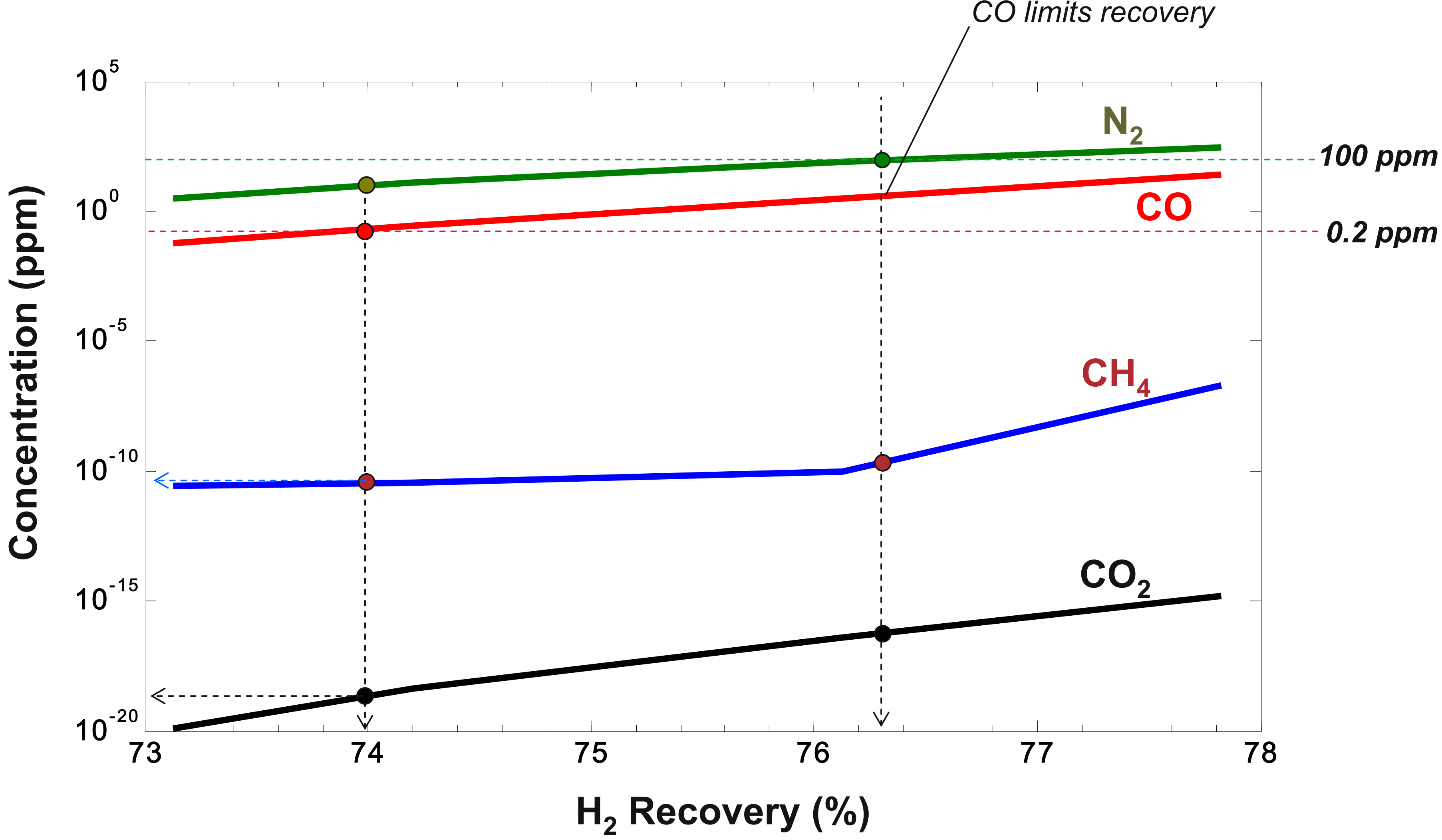
Natural Gas Composition	
CH_4	93.1 %
C_2H_6	3.2 %
C_3H_8	0.7 %
C_4H_{10}	0.4 %
CO_2	1.0 %
N_2	1.6 %

Steam Reformer/ Water-Gas Shift

Reformate Composition	
	S/C = 4
H_2	76.4 %-dry
CH_4	2.8 %-dry
CO_2	17.5 %-dry
CO	2.8 %-dry
N_2	0.4 %-dry
H_2S	100 ppmv

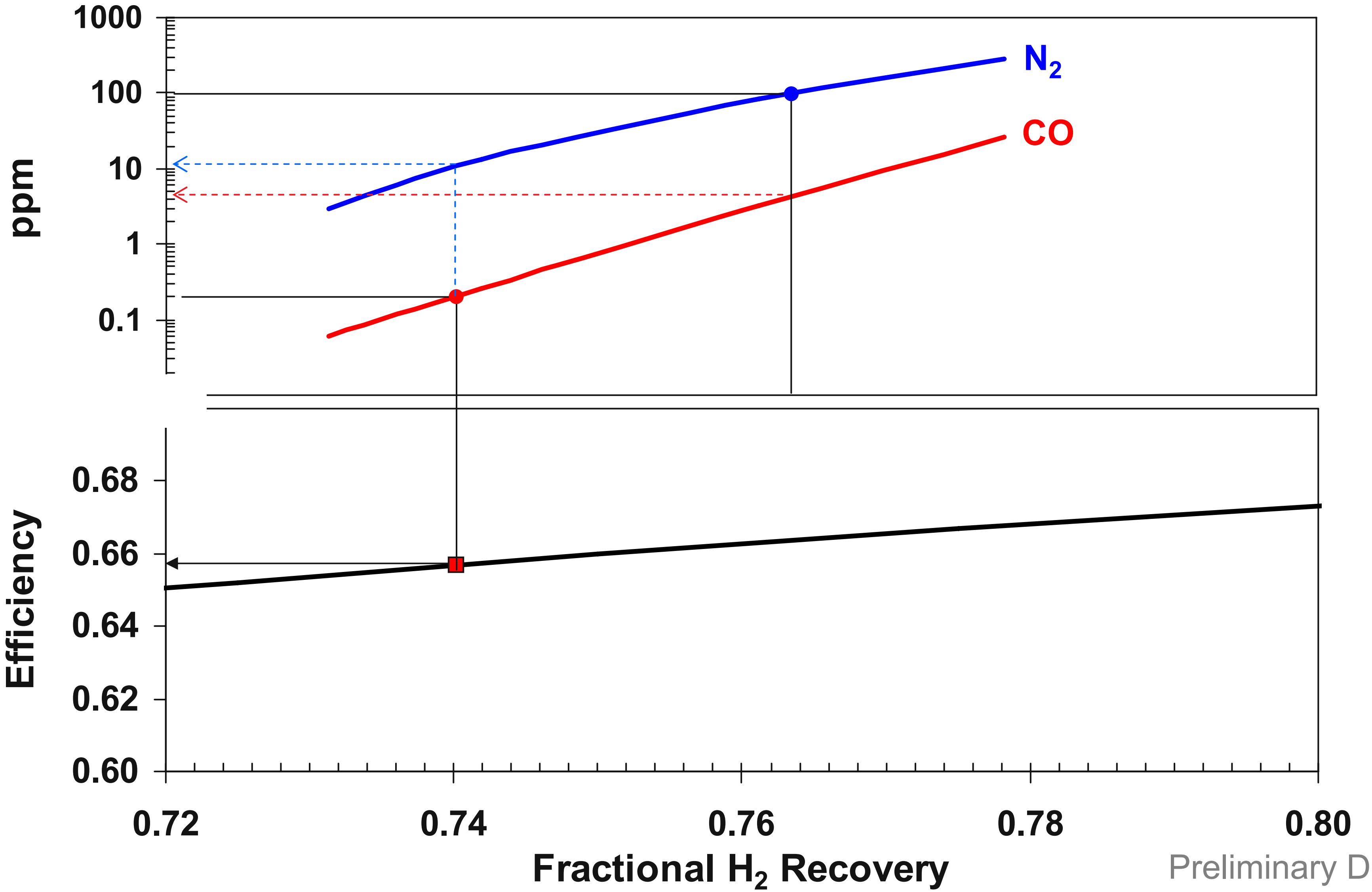
Preliminary Data

For the base case, CH_4, CO_2, and H_2S levels in the product hydrogen are very low



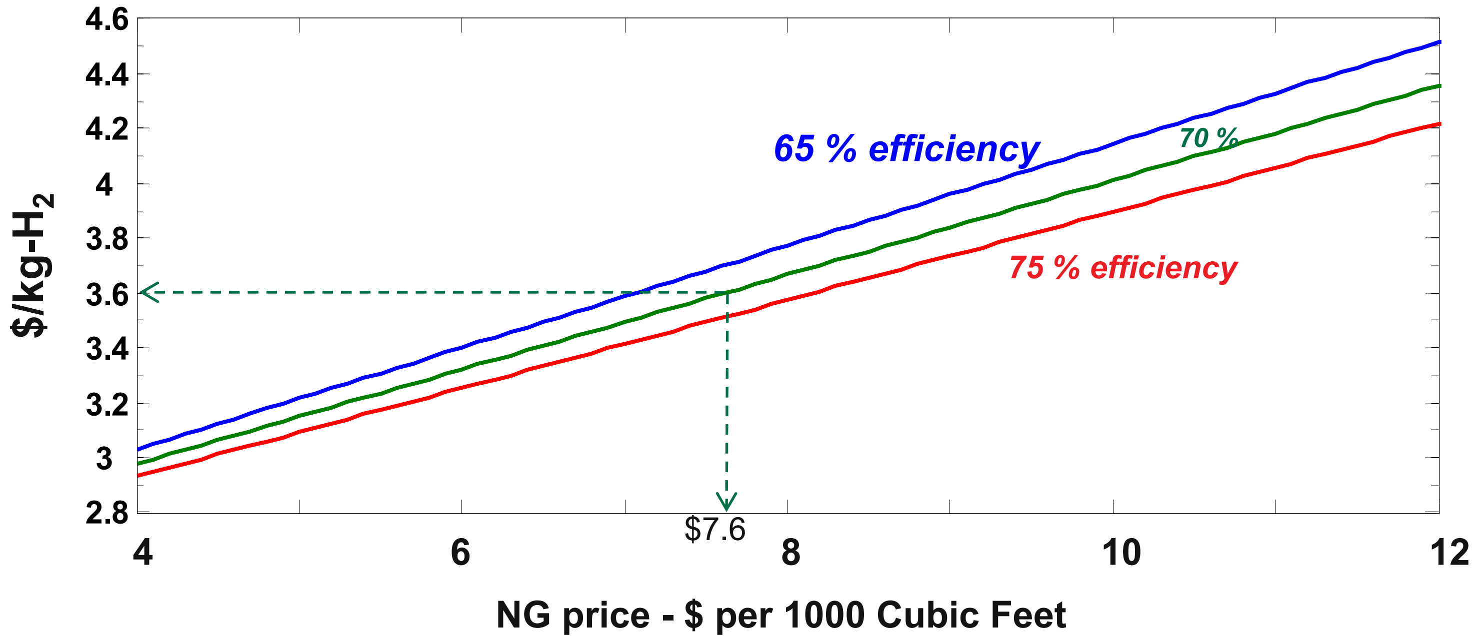
Preliminary Data

CO specification of 0.2 ppm limits the H_2 recovery to 74% and yields an efficiency of 66%



Preliminary Data

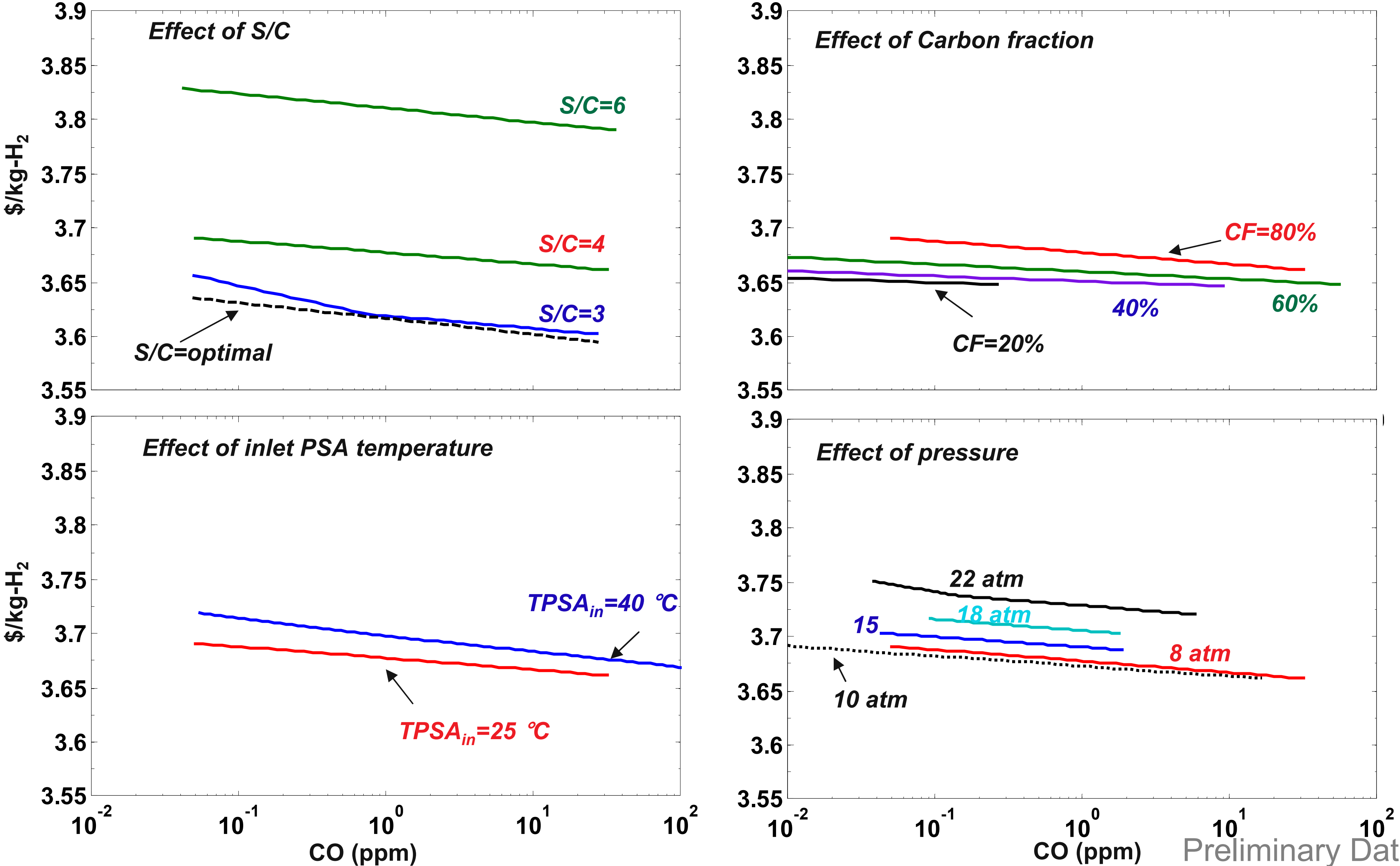
Hydrogen costs as a function of natural gas price and SMR-PSA process efficiency



*Industrial NG Price (EIA average for 2007) = $7.60/1000 cu ft

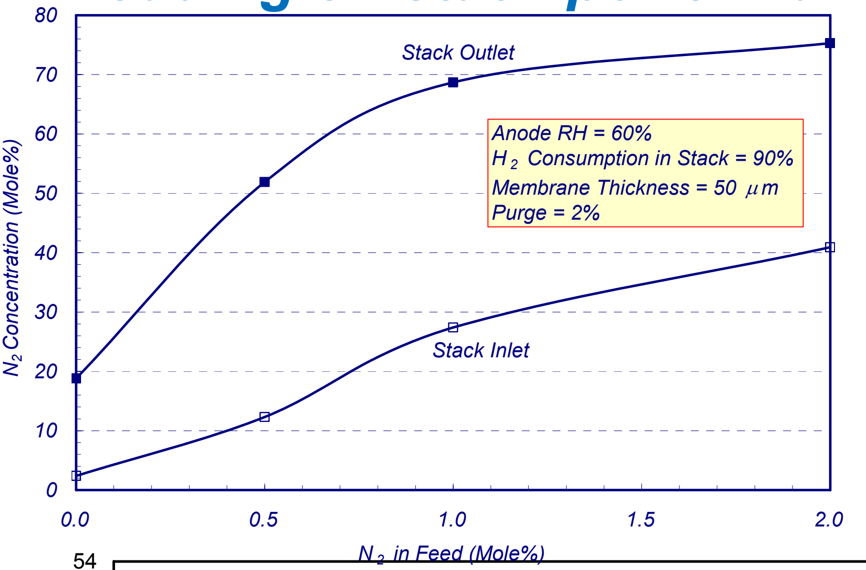
Preliminary Data

Hydrogen cost (by H2A) as a function of CO concentration in H_2 (NG @ \$7.60 / 1000 cu ft)



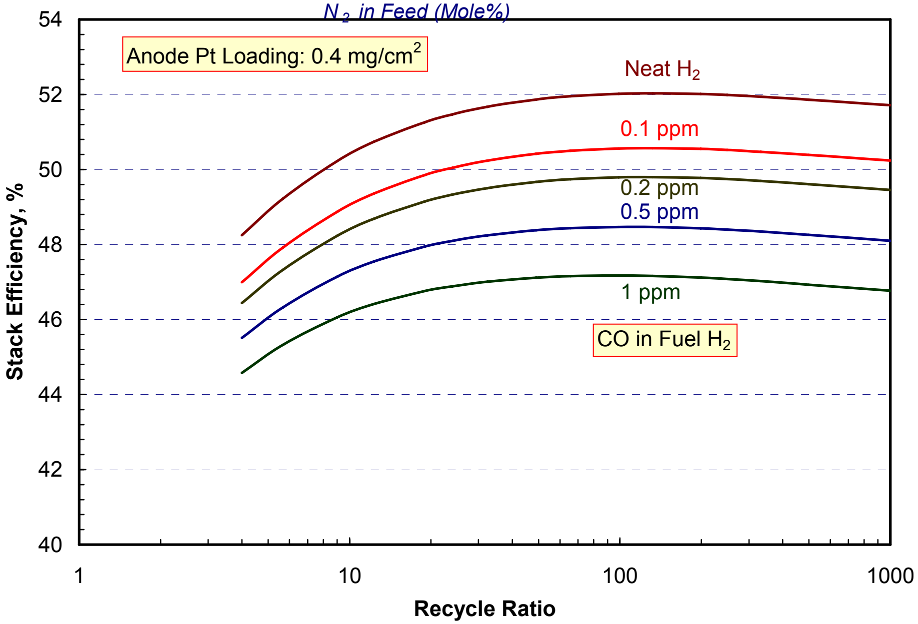
Preliminary Data

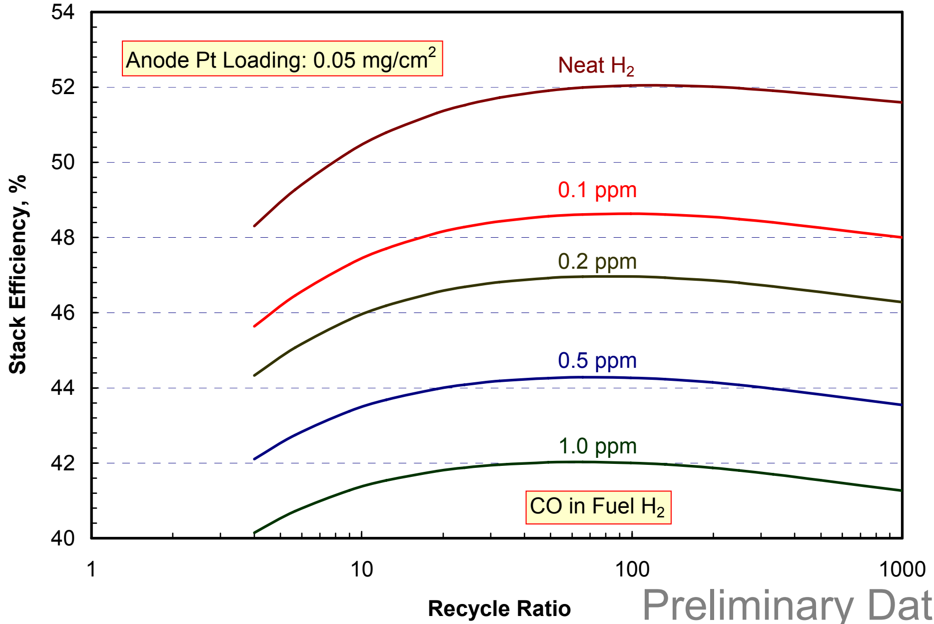
Fuel cell modeling shows the effects of N_2, CO, and Pt loading on stack performance and efficiency



Influence of Pt loading on CO poisoning

Pt Loading	0.4 mg/cm^2		0.05 mg/cm^2	
CO, ppm	ΔV	Δη	ΔV	Δη
0.1	18.4	1.5	42.3	3.4
0.2	28.1	2.2	63.3	5.1
0.5	44.1	3.6	95.9	7.8
1.0	60.5	4.9	124.3	10.0





Preliminary Data

Such analyses can be combined with fuel cell system performance to assess overall lifecycle costs

Example: Effect of CO concentration in fuel H_2

CO concentration in H_2	ppm	0.1	0.2	0.5	1.0
Cost of H_2	$/kg	3.630	3.627	3.621	3.617
Fuel cell stack efficiency	% (LHV)	50.7	49.4	47.8	46.4
FCV/ICEV[1] fuel econ. multiplier		2.54	2.50	2.46	2.42
Fuel economy	mpgge	50.8	50.0	49.2	48.4
H_2 required (for 100,000 miles)	kg	1,970	1,998	2,033	2,065
Cost of fuel (for 100,000 miles)	$	7,152	7,246	7,361	7,467

[1] SUV type ICEV achieving 20 mpg

Preliminary Data

Finally, fuel quality verification is likely to add several ¢/kg (per contaminant analyzed) to H_2 costs

CO Concentration in H_2	ppm	0.2	0.5	1.0
Grab Samples, Off-Line Analysis				
Analytical cost (per analysis)	$	150	150	150
Interval between analyses	days	1	1	1
Plant capacity	kg/day	1500	1500	1500
Cost of Analysis	$/kg	0.100	0.100	0.100
On-Line Instrumental Analysis (for each contaminant)				
Instrument cost	$	10^5	10^5	0.5 x10^5
Instrument life	years	5	5	5
Operation / maintenance	$/year	3000	3000	3000
Cost of Analysis	$/kg	0.043	0.043	0.024

Preliminary Data

Summary

- Draft Roadmap submitted to DOE
  - species-specific data summaries in the Appendices have been used by SAE in their deliberations on revising the TIR J-2719
  - workshops and meetings used to bring fuel cell developers and fuel providers together

- PSA model set up to correlate impurity concentrations with H_2 recovery and production efficiency
  - used S/C, pressure, PSA inlet temperature, and sorbent proportions as key parameters
  - results used with H2A to evaluate impacts of fuel quality requirements on hydrogen costs

- Modeling of impurity effects on fuel cell performance is being used to assess impacts on costs

Future work

- Further develop the PSA model and obtain results for
  - natural gas, ethanol, and other feedstocks of interest
  - electrolysis-derived H_2
  - verifying CO or other species as viable canary species
  - determining composition bandwidth over which other species remain at or below proposed allowable limits
- Use fuel cell impurity modeling data to develop relationships between contaminant levels and fuel cell costs, including efficiency and durability
  - for CO, CO_2, H_2S / COS, NH_3, condensable hydrocarbons
- Update cost analyses with new data and validated modeling results for H_2 purification, drive-cycle fuel cell performance, and off-line and on-line analyses for quality verification
- Continue working with H2QWG, ISO/SAE, etc., and organize related workshops to bring together fuel providers with fuel users to promote ongoing dialogue and identify key results and data needs