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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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U.S. Department  
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# Overview

## Timeline

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

## Budget

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

## Barriers

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

## 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

Month-Year	Milestone
Nov-07	Identify one or more R&D areas to fill a gap in critical information <i>Hydrogen sampling and analysis for quality verification identified as a major challenge (technology, cost)</i>
Dec-07	Establish hydrogen purification cost versus contaminant level for four contaminant species <i>SMR-PSA model has been developed and preliminary results discussed in several forums</i>
Aug-08	Develop quantitative models for lifecycle costs of fuel cell vehicles (including the cost of H <sub>2</sub> ) versus contaminant level for four contaminant species <i>Results of impurity effects modeling of fuel cell performance will be used to assess effects on fuel cell costs</i>

# 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<sub>2</sub> 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<sub>2</sub>
- Developed methodology to evaluate cost effects using H2A

# Developing the SMR-PSA performance model

- Plant Size : 1,500 kg/day of H<sub>2</sub> 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

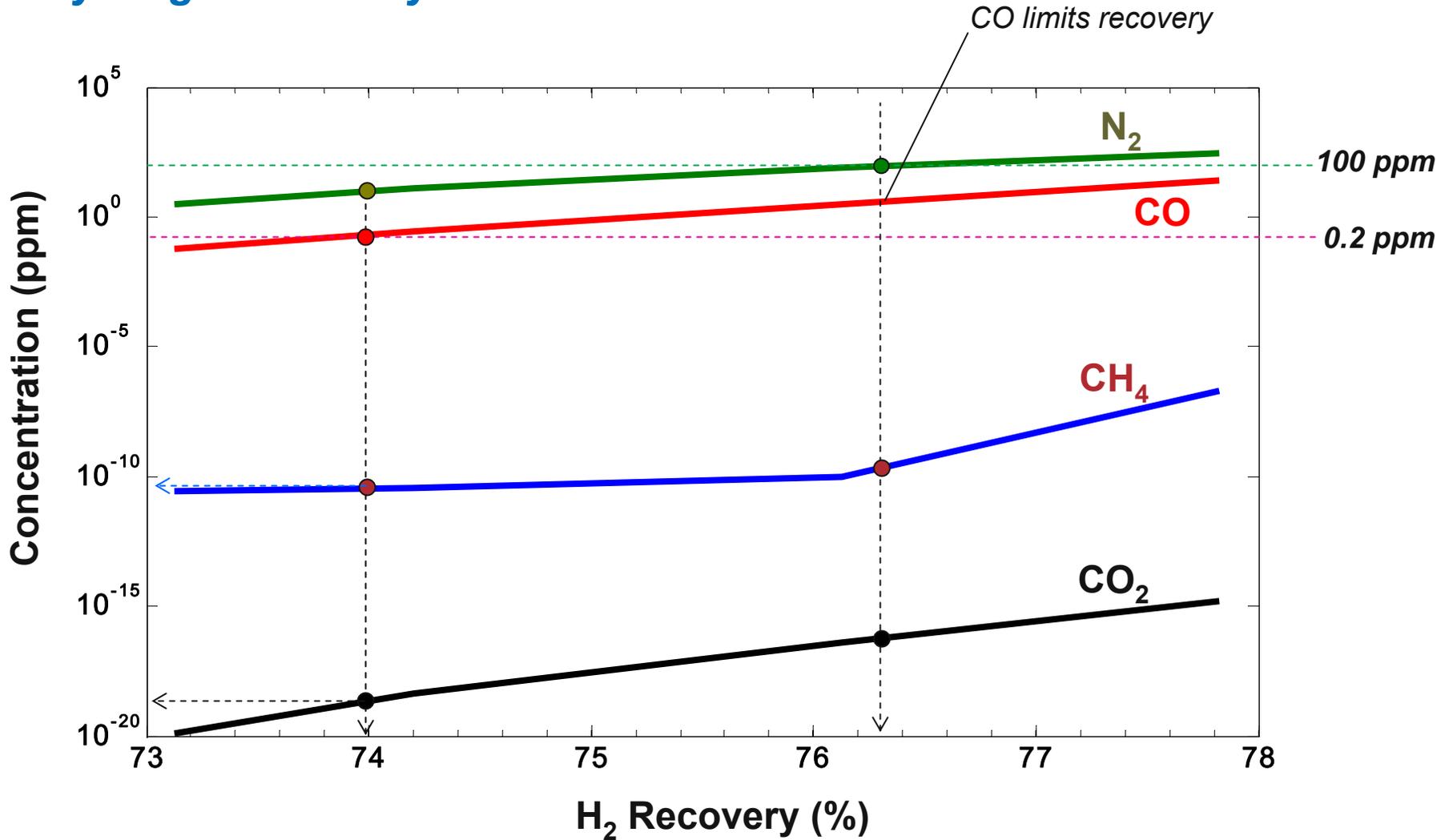
Natural Gas Composition	
CH <sub>4</sub>	93.1 %
C <sub>2</sub> H <sub>6</sub>	3.2 %
C <sub>3</sub> H <sub>8</sub>	0.7 %
C <sub>4</sub> H <sub>10</sub>	0.4 %
CO <sub>2</sub>	1.0 %
N <sub>2</sub>	1.6 %



Reformat Composition	
S/C = 4	
H <sub>2</sub>	76.4 %-dry
CH <sub>4</sub>	2.8 %-dry
CO <sub>2</sub>	17.5 %-dry
CO	2.8 %-dry
N <sub>2</sub>	0.4 %-dry
H <sub>2</sub> S	100 ppmv

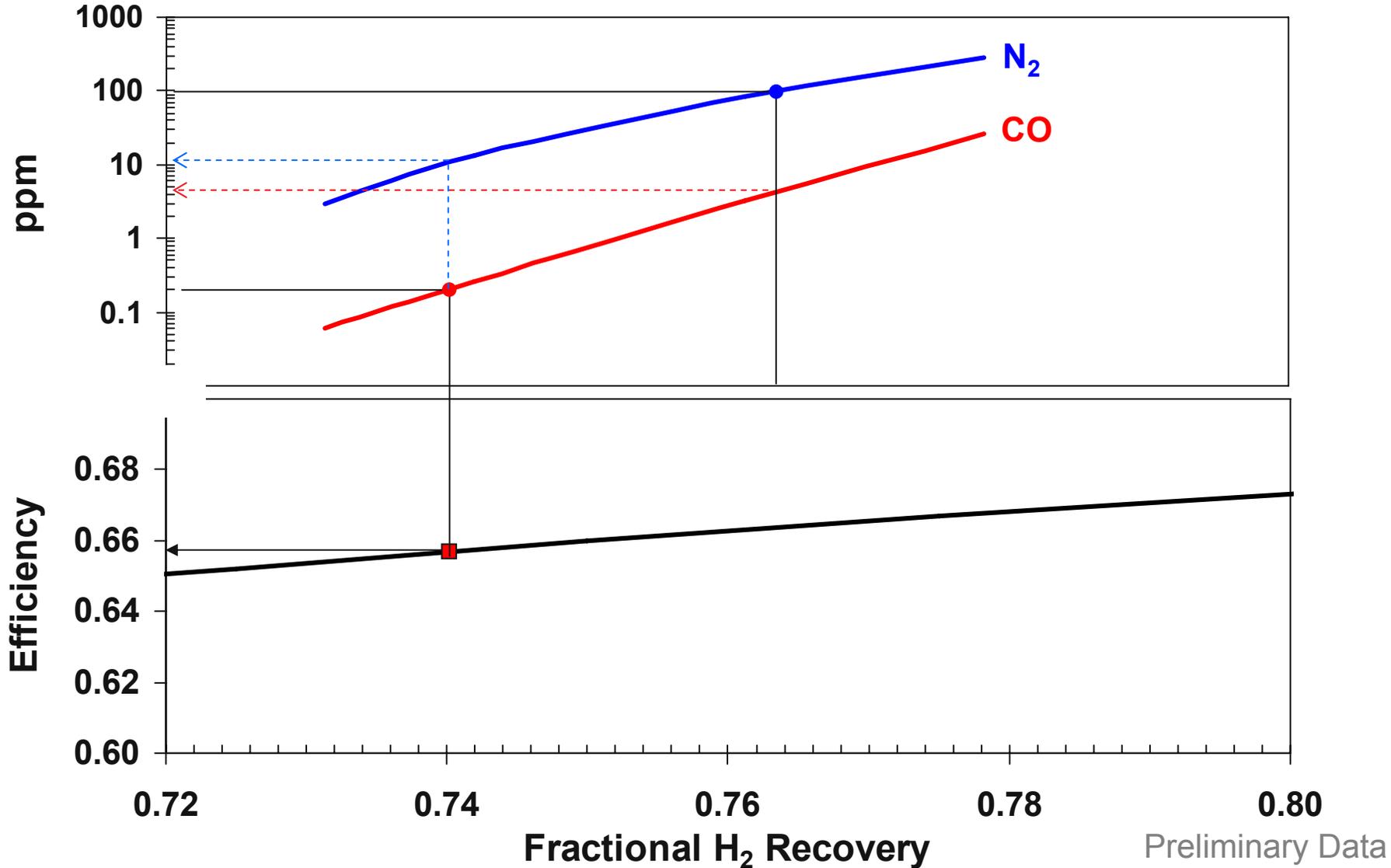
Preliminary Data

For the base case,  $\text{CH}_4$ ,  $\text{CO}_2$ , and  $\text{H}_2\text{S}$  levels in the product hydrogen are very low



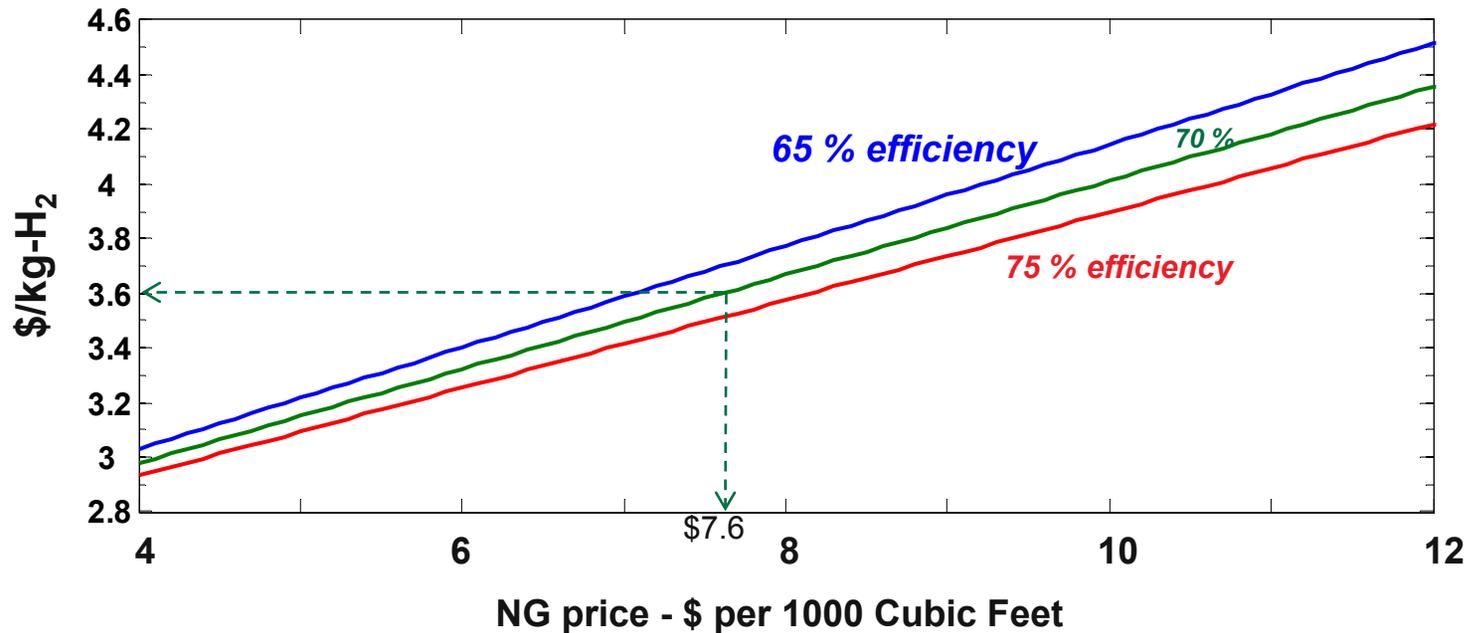
Preliminary Data

*CO specification of 0.2 ppm limits the H<sub>2</sub> recovery to 74% and yields an efficiency of 66%*



Preliminary Data

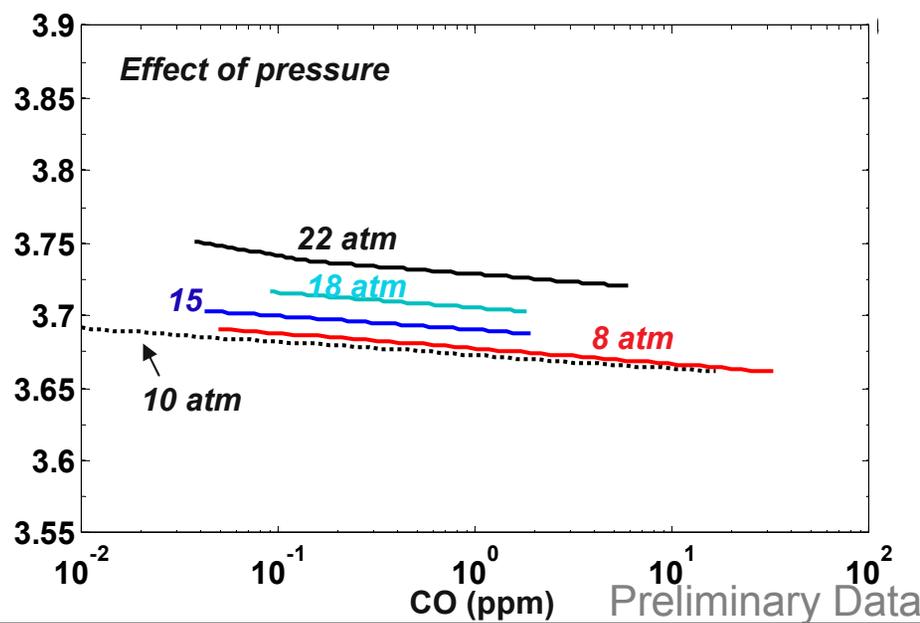
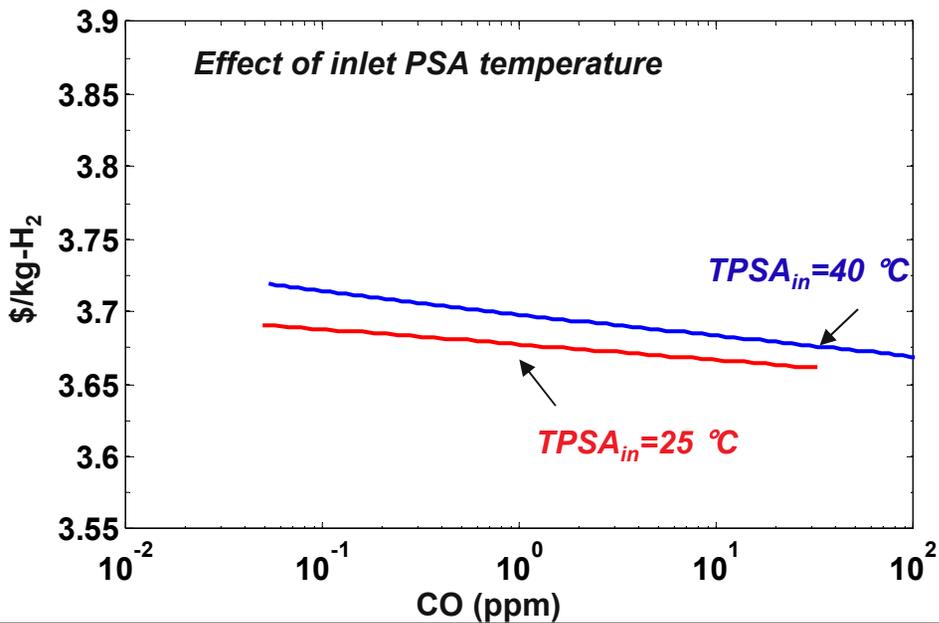
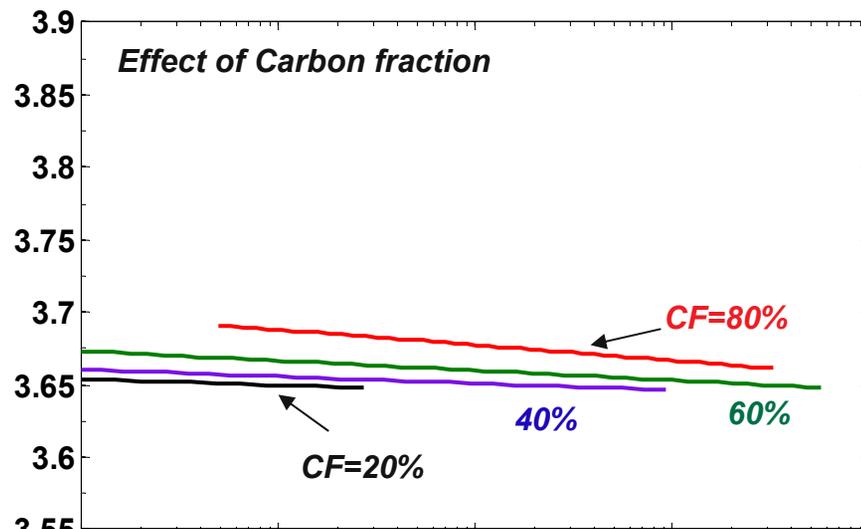
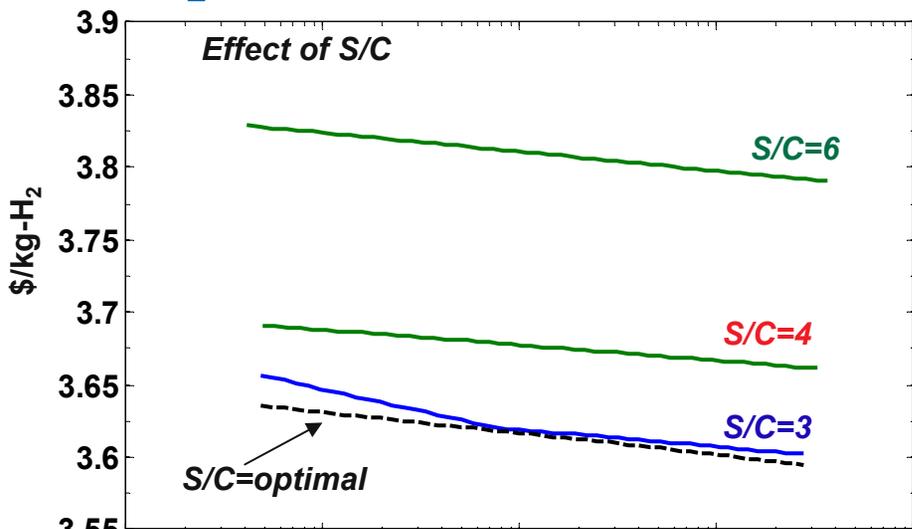
# Hydrogen costs as a function of natural gas price and SMR-PSA process efficiency



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

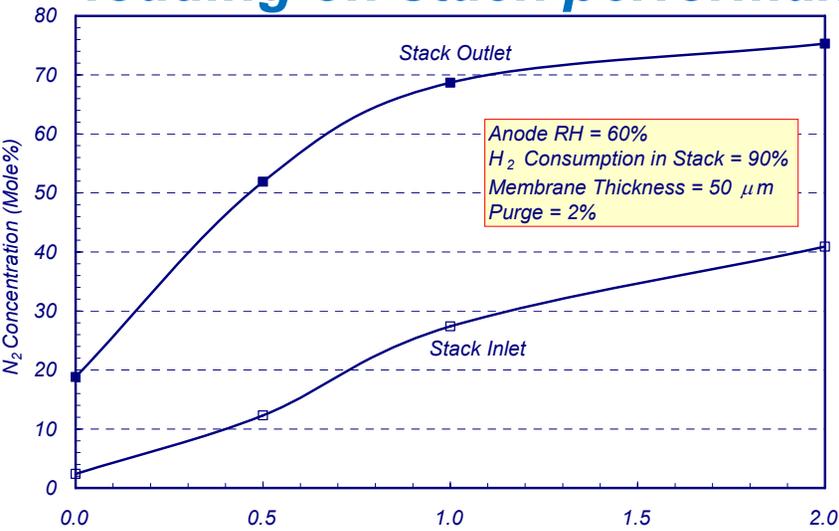
Preliminary Data

# Hydrogen cost (by H<sub>2</sub>A) as a function of CO concentration in H<sub>2</sub> (NG @ \$7.60 / 1000 cu ft)



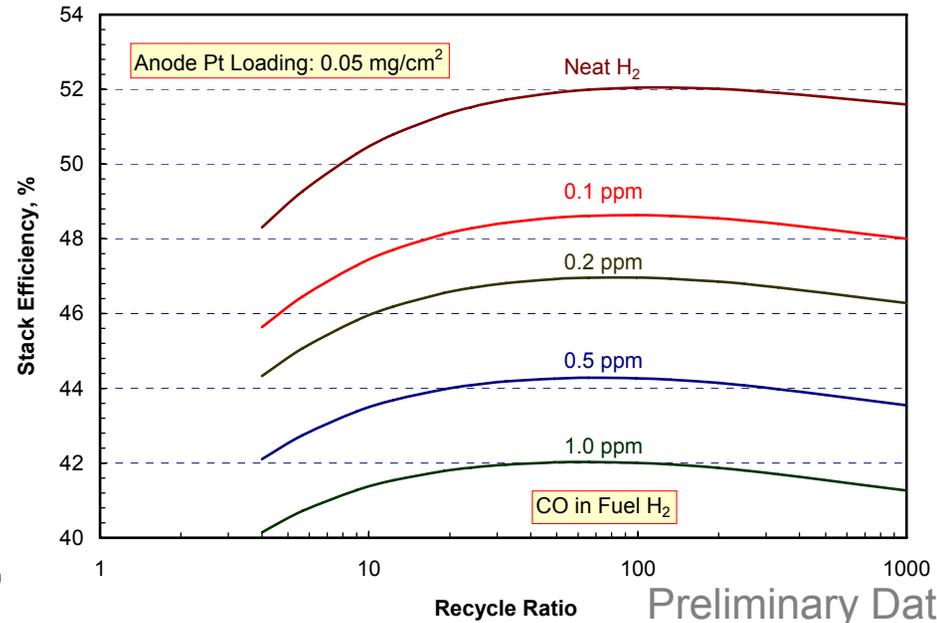
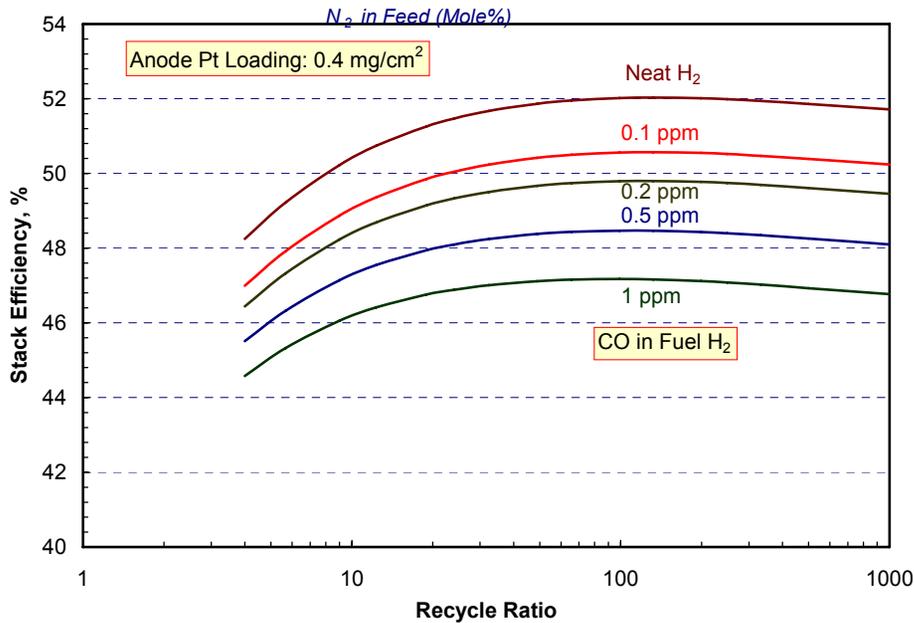
Preliminary Data

# 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

CO, ppm	0.4 mg/cm <sup>2</sup>		0.05 mg/cm <sup>2</sup>	
	$\Delta V$	$\Delta \eta$	$\Delta V$	$\Delta \eta$
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<sub>2</sub>

CO concentration in H <sub>2</sub>	ppm	0.1	0.2	0.5	1.0
Cost of H <sub>2</sub>	\$/kg	3.630	3.627	3.621	3.617
Fuel cell stack efficiency	% (LHV)	50.7	49.4	47.8	46.4
FCV/ICEV <sup>1</sup> fuel econ. multiplier		2.54	2.50	2.46	2.42
Fuel economy	mpgge	50.8	50.0	49.2	48.4
H <sub>2</sub> 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

<sup>1</sup>SUV type ICEV achieving 20 mpg

Preliminary Data

## Finally, fuel quality verification is likely to add several ¢/kg (per contaminant analyzed) to H<sub>2</sub> costs

CO Concentration in H <sub>2</sub>	ppm	0.2	0.5	1.0
<i>Grab Samples, Off-Line Analysis</i>				
Analytical cost (per analysis)	\$	150	150	150
Interval between analyses	days	1	1	1
Plant capacity	kg/day	1500	1500	1500
<b>Cost of Analysis</b>	<b>\$/kg</b>	<b>0.100</b>	<b>0.100</b>	<b>0.100</b>
<i>On-Line Instrumental Analysis (for each contaminant)</i>				
Instrument cost	\$	10 <sup>5</sup>	10 <sup>5</sup>	0.5 x10 <sup>5</sup>
Instrument life	years	5	5	5
Operation / maintenance	\$/year	3000	3000	3000
<b>Cost of Analysis</b>	<b>\$/kg</b>	<b>0.043</b>	<b>0.043</b>	<b>0.024</b>

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<sub>2</sub> 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<sub>2</sub>
  - 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<sub>2</sub>, H<sub>2</sub>S / COS, NH<sub>3</sub>, condensable hydrocarbons
- Update cost analyses with new data and validated modeling results for H<sub>2</sub> 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