DOE – Hydrogen, Fuel Cells, and Infrastructure Technologies

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DOE Hydrogen, Fuel Cells, and Infrastructure Technologies Program

Systems Analysis Workshop

July 28-29, 2004

Washington, D.C.

HFCI Analysis

- National Laboratory projects (including subcontracts to National Labs) – covered by presentations later today.
- Cooperative Agreements
  - GTI – Sunita Satyapal
  - Battelle – Kathi Epping
  - TIAX – Roxanne Danz

GTI Project

Development of Cost-Effective and Reliable Underground Off-Board Hydrogen Storage Technology

- Gas Technology Institute (GTI)
  - Over 40 years RD&D in hydrogen technologies

GTI Hydrogen Capabilities and Activities

- Hydrogen Production (reformation, gasification, thermochemical, thermal decomposition, biological, and electrolysis)
- Gas Processing (clean-up, purification, liquefaction, and chemical processing such as gas-to-liquids conversions)
- Distribution and Handling (pipeline operations, metering/measurement, materials compatibility, permeation and leakage, compression, storage, etc.)
- End Uses (fuel cells, engines, turbines, industrial processes, appliances)
- Market Research (market investigations, business analysis)
- Vehicles: Integrated hydrogen fuel stations, fuel dispensing, hydrogen storage, and fuel cell components for vehicles
- Codes & Standards: Participation in SAE and other pertinent code, standards, and recommended practices

GTI- Off-board H_2 Storage Project

Subcontract:

- NexGen Fueling
  - Division of Chart Industries- one of the world's largest and most technically advanced LNG infrastructure supplier; $325M sales in NexGen Fueling division
  - A leading manufacturer of cryogenic systems and components worldwide, including on-board and bulk cryogenic tanks and a variety cryogenic pumps and vaporizers

- Principal Investigators
  - Louis A. Lautman (GTI)
    - Manager, Advanced Energy Systems
  - Claus Emmer (NexGen)
    - *Sr. Systems Engineer, > 30 yrs experience (cryogenic vessels)*

New project in response to Hydrogen Storage "Grand Challenge" solicitation…

GTI- Off-board H_2 Storage Project

Project Objectives:

Task 1) Off-board Storage Technology Analysis

- Evaluation of design, cost, operational characteristics of conventional hydrogen storage (high P) vs. LH2 underground storage (~ 6 mo-1 yr)
  - System footprint, capacity, heat gain, leak rates, codes/safety regulations, etc.

Task 2) Off-board Storage Testing & Analysis

- Installation, burial & testing of tank for off-board storage (yrs 2-3)
  - Heat loss tests, soil moisture effect, tank corrosion monitoring, temperature effects, tank vacuum loss, safety monitoring, etc.

Funding:

- DOE $1M (Total ~$1.5M with cost share) over 3 yrs

Project will start Fall 2004 (subject to congressional appropriations)

Scope of work under negotiation: Will include analysis of high P tanks

Skill Set – Capabilities Summary
GTI Project

TYPE OF ANALYSIS	RESIDENT CAPABILITY?	STUDIES SPECIFIC TO H_2?	MODELS SPECIFIC TO H_2?
Resource Analysis	Yes	Yes	
Technoeconomic Analysis	Yes	Yes	
Environmental Analysis	Yes	Yes	
Delivery Analysis	Yes	Yes	
Infrastructure Development Analysis	Yes	Yes	
Energy Market Analysis	Yes	Yes	

Skill Set – People (Battelle)

Battelle Team: Economic Analysis of Stationary PEM Fuel Cell Systems

- **Harry Stone, Economist and Principal Investigator, Battelle – Cincinnati**
- **Darrell Paul, Project Manager, Battelle -- Columbus**
- **Steve Millett, Futurist, Battelle – Columbus**
- **Gretchen Hund, Stakeholder Involvement, Battelle – Seattle**
- **Kathya Mahadevan, Analyst, Battelle – Columbus**

The above staff comprise the core team working on the current DOE project, but many other Battelle staff members are brought onboard for a limited time when there expertise is needed.

Skill Set – Models (Battelle)

Battelle Team: Economic Analysis of Stationary PEM Fuel Cell Systems

Economic analysis of stationary fuel cells and their associated markets to understand the cost targets that will drive the R&D for our program.

- ***<u>Techno-Economic and Lifecycle Cost Models</u>***
  - *Spreadsheet modeling with add-in enhancements to answer "what if" questions*
  - *Model platform: Microsoft Excel, VBA, Crystal Ball*

- ***<u>Interactive Future Simulations (IFS)</u>***
  - *Uses Bayesian probabilities and cross-impact analysis to build models from which an algorithm generates alternative scenarios; modeling and simulation tool*
  - *Model platform: Battelle-initiated software program written in C language for Windows*
  - *Model limitations: best suited for macroscopic analysis of probable outcomes*

Skill Set – Capabilities Summary

(Refer to H_2 Analysis Types – last Slide)

Battelle Team: Economic Analysis of Stationary PEM Fuel Cell Systems

TYPE OF ANALYSIS	RESIDENT CAPABILITY?	STUDIES SPECIFIC TO H_2?	MODELS SPECIFIC TO H_2?
Resource Analysis	Yes	Yes	No
Technoeconomic Analysis	Yes	Yes	Yes
Environmental Analysis	Yes	Yes	No
Delivery Analysis	Yes	No	No
Infrastructure Development Analysis	Yes	No	No
Energy Market Analysis	Yes	Yes	Yes

Analysis Issues (Battelle)

- Stationary Fuel Cells and their associated markets need to be studied to understand the cost targets that drive our program's R&D

- Who will take leadership in the commercialization of hydrogen fuels and under what circumstances?

TIAX

- Over 20 year history
  - Fuel Production Analysis – methanol, ethanol, hydrogen
  - Well-to-Wheels - energy and GHG
  - Manufacturing Cost
  - Societal Impacts – cost/benefit analysis
- Fuel Choice for FCV Analysis (DOE)
- Scenario Study (CAFCP)
- CA Petroleum Dependency Study (CEC/ARB)
- Modeling Studies in the 1990s
  - Process Analysis: methanol and hydrogen from biomass
  - Well-to-Wheels: methanol and hydrogen

Skill Set – People - TIAX

- Peter Teagan – technical and market analysis, EPYX ATR development (1989)
- Stefan Unnasch – well-to-wheels studies (1987), vehicle ownership cost analysis (1986)
- Steve Lasher – integrated hydrogen and fuel cell (PEM and SOFC) system thermodynamic modeling and cost assessments
- Jayanti Sinha – economic models, drive cycle analysis
- Michael Chan – hydrogen transition modeling
- Eric Carlson – economic/cost analysis

Skill Set – Models (TIAX)

- Models that Explicitly Include Hydrogen
  - GREET Post Processor
  - Fuel Cell Vehicle Ownership Cost Model
  - Hydrogen Infrastructure Model
  - Molecular Modeling
  - Fuel Cell System Model Projects

Skill Set – Projects (TIAX)

- Projects that Explicitly Include Hydrogen
  - Fuel Choice for FCV Analysis
    - **Phase I-II: Well-to-Wheel and Ownership Cost** *Completed: February 2002*
    - ***Phase III: Hydrogen Infrastructure Cost*** *Ongoing (different contract than Phases I-II)*
  - Hydrogen Technical Analysis
    - **Phase I: Small-scale Purification Technologies** *Completed: July 2002*
    - **Phase II: Hydrogen Mini-grid** *Ongoing*
  - Manufacturing Cost Study of Automotive PEMFC Fuel Cell System *Ongoing*
  - Analyses of Hydrogen Storage Materials and On-Board Systems *Ongoing*

Skill Set – Models (TIAX)

- <u>Projects that Explicitly Include Hydrogen (con't)</u>
  - Others
    - Energy Efficiency and Emissions of Transportation Fuel Chains
    - The Impact of Electric Vehicles on CO2 Emissions
    - Analysis of Hydrogen Energy Station
    - Development of a Multi-Fuel Reformer
    - Potential PGM Pricing and Availability Barriers to Commercialization
    - Assessment of Fuel Cells as Auxiliary Power Systems for Transportation Vehicles

Skill Set – Capabilities Summary (TIAX)

TYPE OF ANALYSIS	RESIDENT CAPABILITY?	STUDIES SPECIFIC TO H_2?	MODELS SPECIFIC TO H_2?
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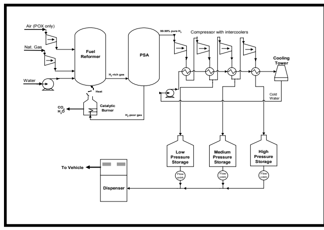
Energy Market Analysis	Yes	Yes	Yes

Backup Slides

Modeling Capabilities Hydrogen Systems (TIAX)

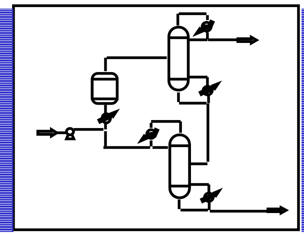
System level modeling and detailed cost databases are used to evaluate hydrogen fuel chain efficiency and overall fuel cost.

Hydrogen Station Conceptual Design



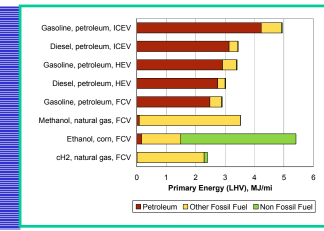
- System layout and equipment requirements

Hydrogen System Process Simulation



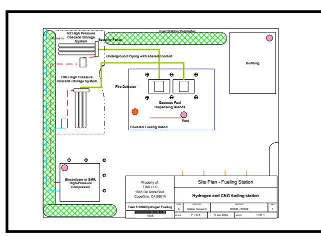
- Energy requirements
- Equipment size/ specs

GREET Post Processor



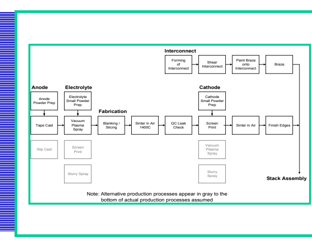
- WTW energy use
- WTW GHG

Site Plans



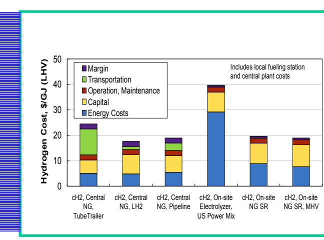
- Safety equipment, site prep, land costs

Equipment Cost Database



- High and low volume equipment costs

Hydrogen Cost Model



- Hydrogen cost (capital, O&M, etc.)

Modeling Capabilities GREET Post Processor (TIAX)

TIAX has developed a GREET Post Processor that enables the effective calculation of energy use and GHG emissions for alternative fueled vehicles.

Highlights

Allows researchers and policy makers to make effective comparisons of different alternative fuel options without the limitations of the GREET model

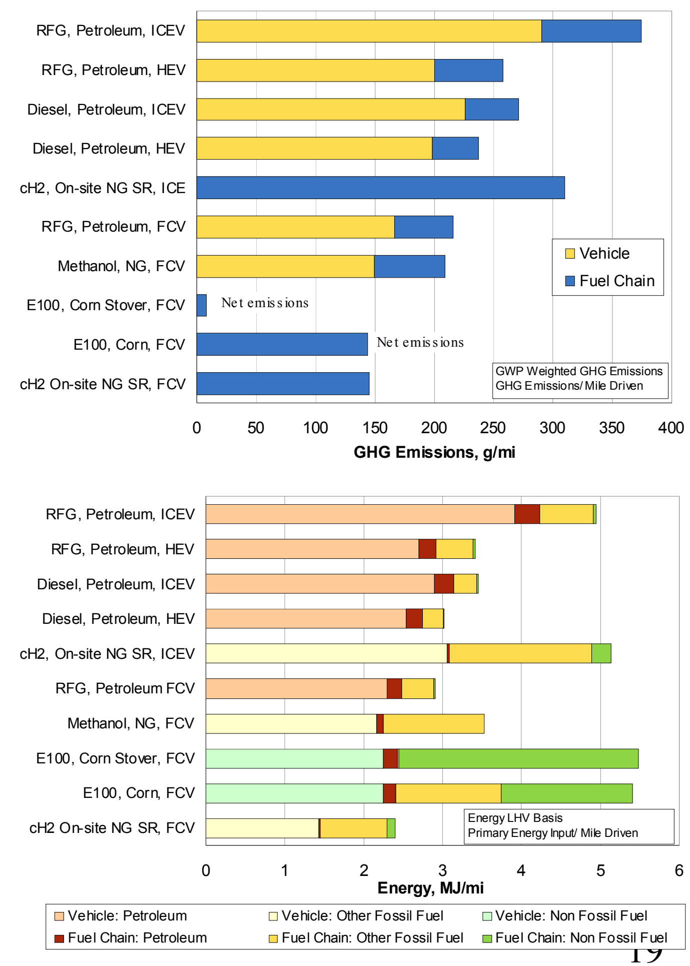
Primary Uses

Provides a user-friendly method of comparing different hydrogen options while exporting the fundamental analysis in the GREET model

External Review

DOE Peer Reviews, ANL, Industry Hydrogen Infrastructure Group (IHIG) and various energy companies

WTW GHG and Energy Use



TIAX has developed a series of modeling tools to evaluate the life cycle cost of fuel cell powered vehicles.

Highlights

The model combines several detailed modeling efforts at TIAX including:

- –Fuel cell stack performance model
- –Fuel cell and hydrogen storage manufacturing cost model
- –Hybrid vehicle cost and performance (i.e., drive-cycle simulation)
- –Hydrogen cost model
- –Vehicle ownership cost model

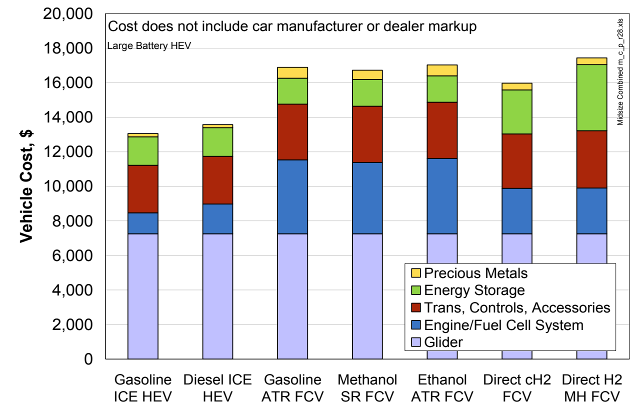
Primary Uses

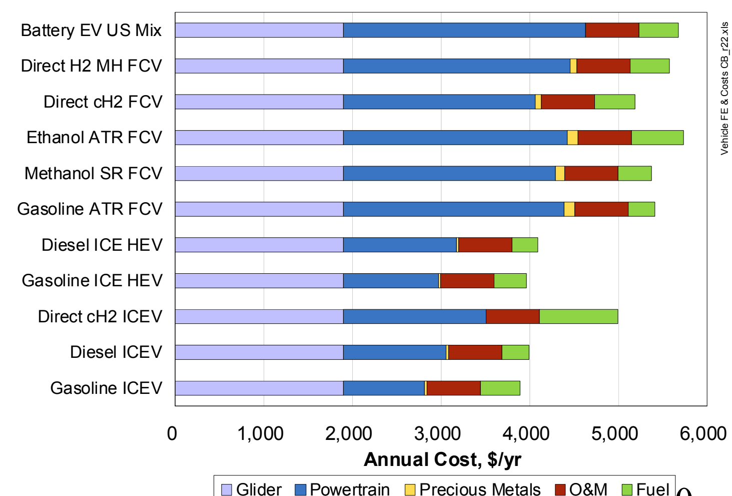
Enables the comparison of the cost of different fuel cell vehicle and technology options

External Review

Vehicle model developed with EPRI HEV working group, fuel cell costs reviewed extensively with fuel cell industry

Vehicle and Ownership Costs





TIAX has developed a hydrogen infrastructure model that evaluates transition strategies for the hydrogen economy.

Highlights

Determines both the capital and operating cost of hydrogen infrastructure introduction options over time

Primary Uses

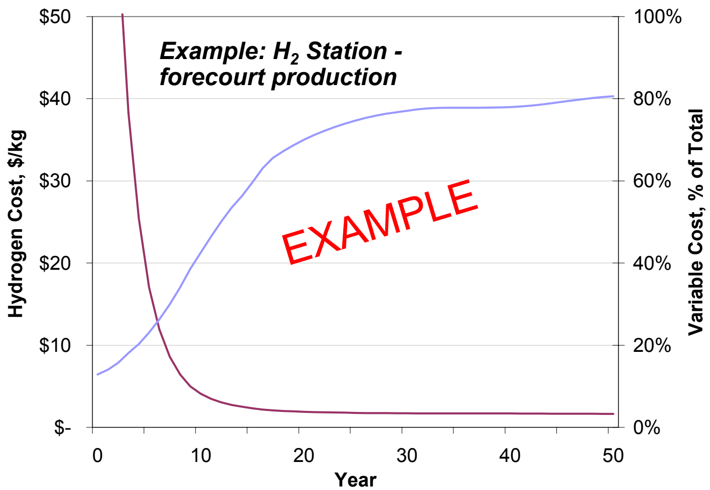
Enables policy makers and investors to assess the capital cost and revenue projections for different hydrogen vehicle and infrastructure build-up scenarios

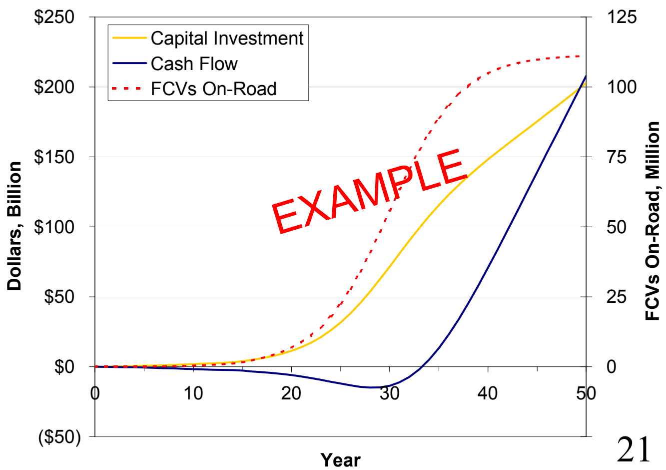
- –Vehicle introduction scenarios; including quick versus long build-up, hydrogen ICEVs
- –Fueling strategies; including central versus local production, mobile fuelers, energy stations

External Review

DOE and CAFCP Peer Reviews, Industry Hydrogen Infrastructure Group (IHIG) and various energy companies

Hydrogen Cost and Cash Flow

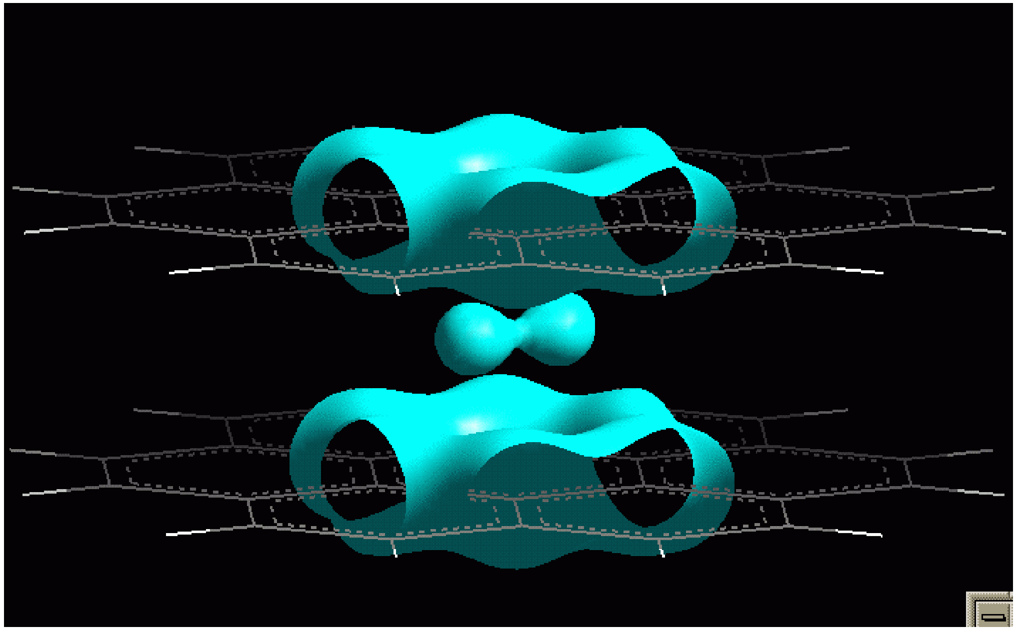




Modeling Capabilities Molecular Modeling (TIAX)

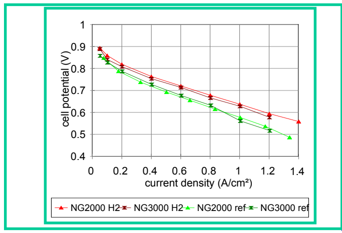
In a previous study of hydrogen storage, we modeled a hydrogen molecule between two graphitic planes to assess hydrogen affinity to this structure.

- We found that, although there is some electron charge transfer from the graphite to the H_2 molecule, there is no localization potential pinning the hydrogen molecule
- We saw that any charge transfer in or out of the graphitic planes results in a decrease of the in-plane lattice vector's magnitude



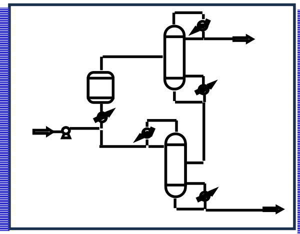
A similar modeling approach is taken to evaluate the cost and performance of complete fuel cell systems.

Stack Performance Model



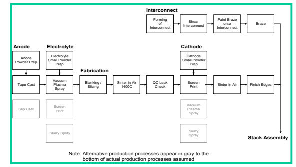
- Power density
- Stack dimensions

Fuel Cell System Process Simulation



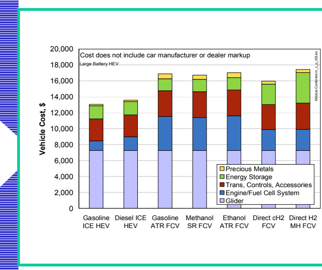
- Equipment size/ specs
- Efficiency

Manufacturing Cost Model



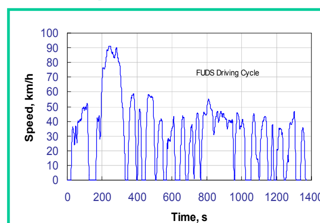
- Fuel cell cost
- Fuel cell weight

Vehicle Ownership Cost Model



- Vehicle manufactured cost
- Ownership cost (vehicle, fuel, O&M)

Drive Cycle Simulation



- Vehicle power
- Fuel economy

Modeling Capabilities Fundamental Stack Model (TIAX)

Fundamental models, such as our PEM stack model, allow us to estimate performance over a wide range of conditions.

Highlights

- Accurate performance valid over a wide range of operating conditions because the model includes fundamental descriptions of important phenomena
  - –Elementary reactions based on current, fundamental understanding
  - –Kinetic parameters, not fitted to data, but obtained from fundamental measurements and calculations in the literature

Primary Uses

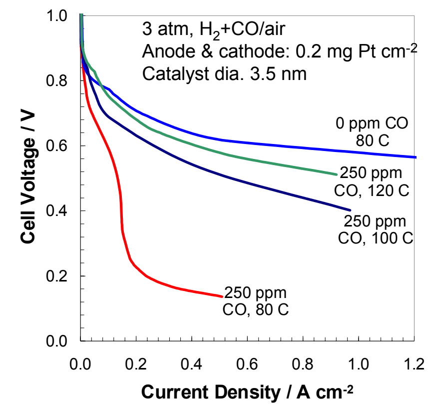
- Estimate cell performance under real and hypothetical scenarios
- Check validity of performance assertions
- Identify and test operating strategies that optimize performance
- E.g., automotive PEMFC

Steady State and Transient Effect of Poisons

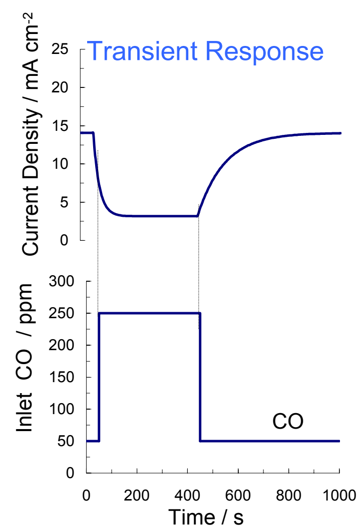
Elementary Reactions

$H_2Pt + Pt = 2\ HPt$
$H_2 + Pt = H_2Pt$
$H_2O + Pt = H_2OPt$
$CO + Pt = COPt$
$COPt + OHPt = CO_2 + HPt + Pt$
$HPt = H + Pt$
$H_2OPt = H + OHPt$
$HPt + OPt = OHPt + Pt$
$H_2OPt + OPt = 2\ OHPt$
$HPt + OHPt = H_2OPt + Pt$
$O_2 + Pt = O_2Pt$
$O_2Pt + Pt = 2\ OPt$
$COPt + OPt = CO_2 + 2\ Pt$

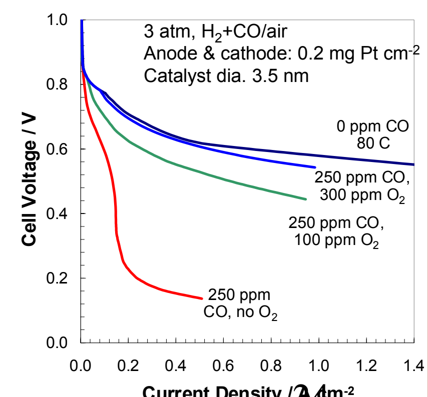
Effect of Temperature



Transient Response



Effect of Air Bleed



Our manufacturing cost model is critical in determining the bottoms-up cost of many hydrogen and fuel cell components.

The Challenge

The OATT wanted to develop an independent cost analysis of a fuel flexible PEMFC system for transportation with which to gauge progress toward PNGV cost targets and to project future cost.

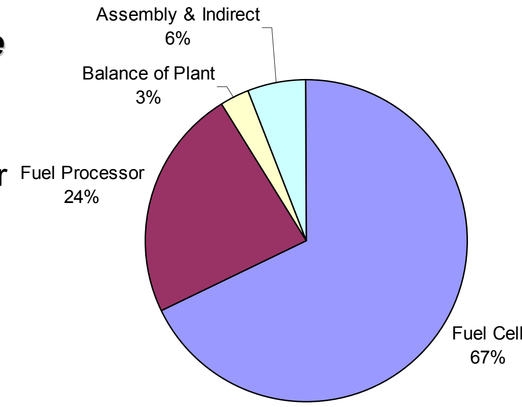
TIAX's Approach

- Develop a system configuration for automotive applications
    - Worked with ANL to construct system design
- Develop an activities based cost model for high volume production (500,000 vehicles per year)
- Present results and assumptions to industry
- Revise model based on feedback from industry
- Use kinetic modeling to provide basis for long term projection

Cost Model Results

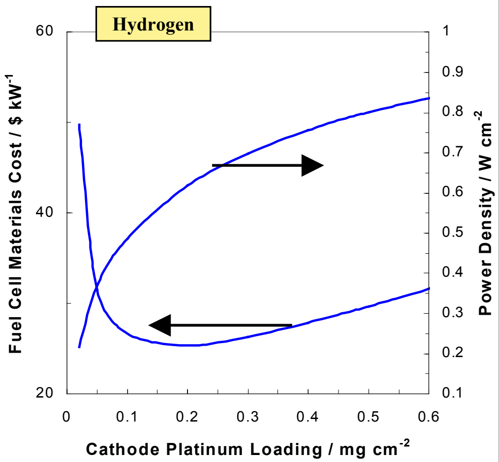
2001 Baseline Cost:

- $324/kW
- 500,000 veh/yr
- fuel flexible reformer (gasoline)



Pt Loading Analysis:

- Based on kinetic analysis
- High temperature membrane
- 0.8V at rated power
- Considers stack resistance



Fuel Choice for FCV Analysis (TIAX)

- **Phase I-II: Well-to-Wheel and Ownership Cost**
  - Completed: February 2002
  - Evaluated well-to-wheel energy use, greenhouse gas emissions, and ownership costs for various PEM FCV fuel options using detailed fuel chain and vehicle performance models and cost analyses. Also evaluated the technology development, commercialization, environmental, safety and other issues surrounding various fuel options and strategies for FCVs. Based on the results, helped DOE develop R&D targets for off-board hydrogen production and provided insight to potential FCV ownership costs for the various options.
- **Phase III: Hydrogen Infrastructure Cost**
  - Ongoing (different contract than Phases I-II)
  - Conducting a net present value analysis on developing a hydrogen infrastructures focusing on the transition from the current situation to various steady-state market penetration cases. Based on the results, will compare financial and other risks to society and individual stakeholders for various transition strategies and propose pathways that minimize risks.

Hydrogen Technical Analysis

(TIAX)

- **Phase I: Small-scale Purification Technologies**
  - Completed: July 2002
  - Evaluated three alternative purification technologies with promising characteristics for small-scale production at hydrogen fueling stations using detailed process models and cost analyses of various system configurations, including: high and low pressure autothermal and steam reforming, and high and low pressure hydrogen storage. Based on the results, determined the most promising purification technologies compared to conventional pressure swing adsorption in terms of overall system efficiency and cost to produce hydrogen.
- **Phase II: Hydrogen Mini-grid**
  - Ongoing
  - Evaluating the feasibility of hydrogen production for both vehicle fueling and distributed fuel cell power using short distance hydrogen transmission (a.k.a. hydrogen mini-grid) via compressed hydrogen and metal hydride slurry. Detailed cost analysis and process modeling are being used to determine the overall cost, energy use, and emissions benefits of the mini-grid strategies compared to stand-alone and conventional systems.

Manufacturing Cost Study of Automotive PEM FC Fuel Cell System (TIAX)

- Ongoing
- In conjunction with Argonne National Labs, have developed detailed designs for both on-board reforming and direct hydrogen automotive PEMFC systems. Based on the detailed designs, conducted bottoms-up assessment of fabrication costs for 25-100 kW PEMFC systems at both high and low cell voltage designs and vetted the results with numerous developers.

Analyses of Hydrogen Storage Materials and On-Board Systems (TIAX)

- New Project
- Analysis of various hydrogen storage technologies compared to high P tank baseline
- TIAX will work with a team of industry experts to evaluate several categories of on-board hydrogen storage –
  - Compressed hydrogen
  - Cryogenic and hybrid approaches
  - Reversible on-board storage systems:
    - Metal hydrides
    - Carbon-based materials and high surface area adsorbents
  - Regenerable (off-board) storage systems- e.g. chemical hydrides
- Objectives:
  - Compare the different storage technologies and approaches in terms of system level capacity, capital costs, lifecycle costs, energy efficiency, and environmental impact.

Others (TIAX)

- **Energy Efficiency and Emissions of Transportation Fuel Chains**
  - Evaluated the energy inputs, GHG and criteria pollutant emissions for a variety of fuels including methanol and hydrogen from natural gas, coal, and renewables. Based on the results, assess the feasibility and potential environmental benefits of these fuels for fuel cell vehicle applications.
- **The Impact of Electric Vehicles on CO2 Emissions**
  - Calculated energy and CO2 emissions on a well-to-wheels basis for battery electric, hybrid and conventional ICE vehicles using drivetrain and vehicle performance models. Based on the results, compared the environmental impact of each vehicle choice and recommended pathways to minimize energy use and CO2 emissions.
- **Analysis of Hydrogen Energy Station**
  - Evaluating the feasibility of single source hydrogen production for both vehicle fueling and fuel cell power generation (a.k.a. hydrogen energy station). Will assess the costs and efficiencies for various energy station configurations and investigate potential field-test sites for energy stations with 50kW fuel cells.

Others (con't) (TIAX)

- **Development of a Multi-Fuel Reformer**
  - Aided by in-house kinetic modeling and bench-scale experimental evaluation, designed and tested a novel, compact catalytic partial oxidation reactor. Based on the results, developed and successfully demonstrated fuel cell operation on gasoline reformate which lead to the formation of a spin-off company that continues to develop and also sells fuel processing and fuel cell systems.
- **Design and Testing of Hydrogen Storage Materials**
  - We built a hydrogen storage test facility, which was subsequently used to independently test the performance characteristics of a variety of hydrogen storage technologies, including metal hydrides and carbon nanostructures. Based on the results, we evaluated the feasibility of each storage technology compared to conventional compressed gas and liquid storage.
- **Potential PGM Pricing and Availability Barriers to Commercialization**
  - We developed an econometric model to project the impact of fuel cell commercialization scenarios on platinum price and availability based on historical responses of platinum markets to new application demands. Based on the results, we evaluated platinum pricing and availability effects on the potential commercialization of fuel cells.
- **Assessment of Fuel Cells as Auxiliary Power Systems for Transportation Vehicles** (ongoing)
  - We are investigating various fuel cell APU performance attributes, such as: fuel flexibility, start-up time, power level, duty cycle, weight, volume, cost, and overall vehicle efficiency; using detailed system designs and process models. Based on the results, we will evaluate the viability of PEMFCs and SOFCs as APUs for vehicles and perform a trade-off analysis for the critical design and performance parameters.