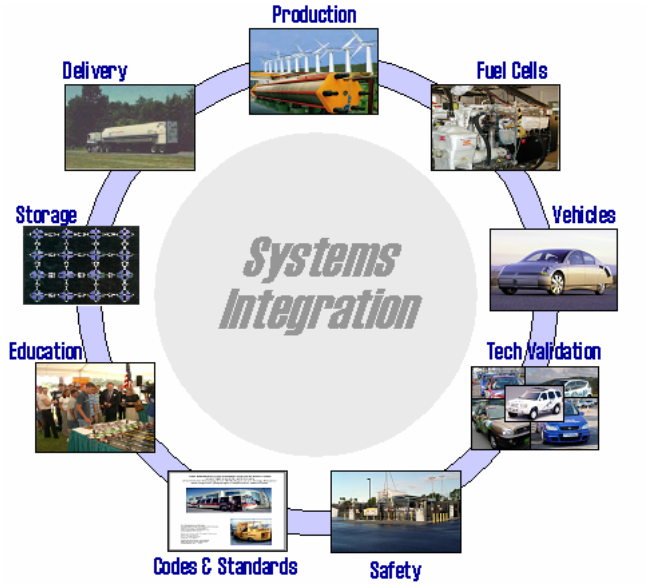
DOE Hydrogen Program

Macro-System Model



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June 11, 2008

Project ID # AN4

This presentation does not contain any proprietary or confidential information

Overview

Timeline

- Start date: Feb 2005
- Completion: Sept 2010
- Percent complete: 35%

Budget

- Total funding:
  - 100% DOE funded
- FY07 funding:
  - $190K NREL/SIO
  - $336K Sandia NL
  - $80K other contracts
- FY08 funding
  - $300K NREL/SIO
  - $340K Sandia NL

Barriers

- Stove-piped/Siloed analytical capability (B)
- Inconsistent data, assumptions and guidelines (C)
- Suite of Models and Tools (D)

Partners

- Sandia National Laboratories (computational development)
- NREL (H2A Production, well-to-wheel analysis validation, HyDRA)
- ANL (HDSAM, GREET, well-to-wheel analysis validation)
- Sentech (Documentation)
- Directed Technologies, Inc (HyPRO)

Project Objectives

- **Overall objectives**
  - Develop a macro-system model (MSM) aimed at
    - Performing rapid cross-cutting analysis
      - Utilizing and linking other models
      - Improving consistency of technology representation (i.e., consistency between models)
    - Supporting decisions regarding programmatic investments and focus of funding through analyses and sensitivity runs
    - Supporting estimates of program outputs and outcomes
- **2007/2008 objectives**
  - Improve structure of the MSM and develop a GUI
  - Update versions of component models
  - Add stochastic analysis capability
  - Validate MSM results
  - Begin interaction between MSM and spatial and temporal models

Approach: MSM Development

Determine Methodology

Input from Analysts & Modelers

- Identify issues the MSM should address
- Define requirements
- Evaluate alternative model architectures

Initial objectives

Proof of concept / Initial analysis

- Identify information to transfer
- Define implicit calculations
- Develop model-linking methodology
- Validate use of models
- Revisit alternatives

Experience

Extensible tool

- Develop & validate extensible & robust structure
- Develop GUI & web interface
- Update MSM with component model updates
- Add stochastic capability
- Provide documentation
- Develop run database

Additional models

Additional Capability

- Revisit analysis issues and MSM requirements
- Select additional models
- Validate use of models
- Develop data-transfer capability

Analysis community interactions

Application

- Use MSM for analysis
- Update models using the MSM
- Meetings to validate approach, methodology, and results

Completed previously

Completed this year

Underway

Future Activities

Earlier Work: Initial Analysis Issues

Financial

What effects could policy and incentives have on transition?

Environmental

How / how much does a hydrogen economy affect the environment?

R&D

ID critical / risky links in potential hydrogen pathways?

Are the current technical targets the best ones? What interdependencies do they have?

How should components and interfaces be optimized?

Transition

Compare potential transition pathways.

ID stumbling blocks that could affect transition paths? Could R&D overcome them?

What impacts could competing technologies have on transition?

What is the emissions profile if hydrogen is used?

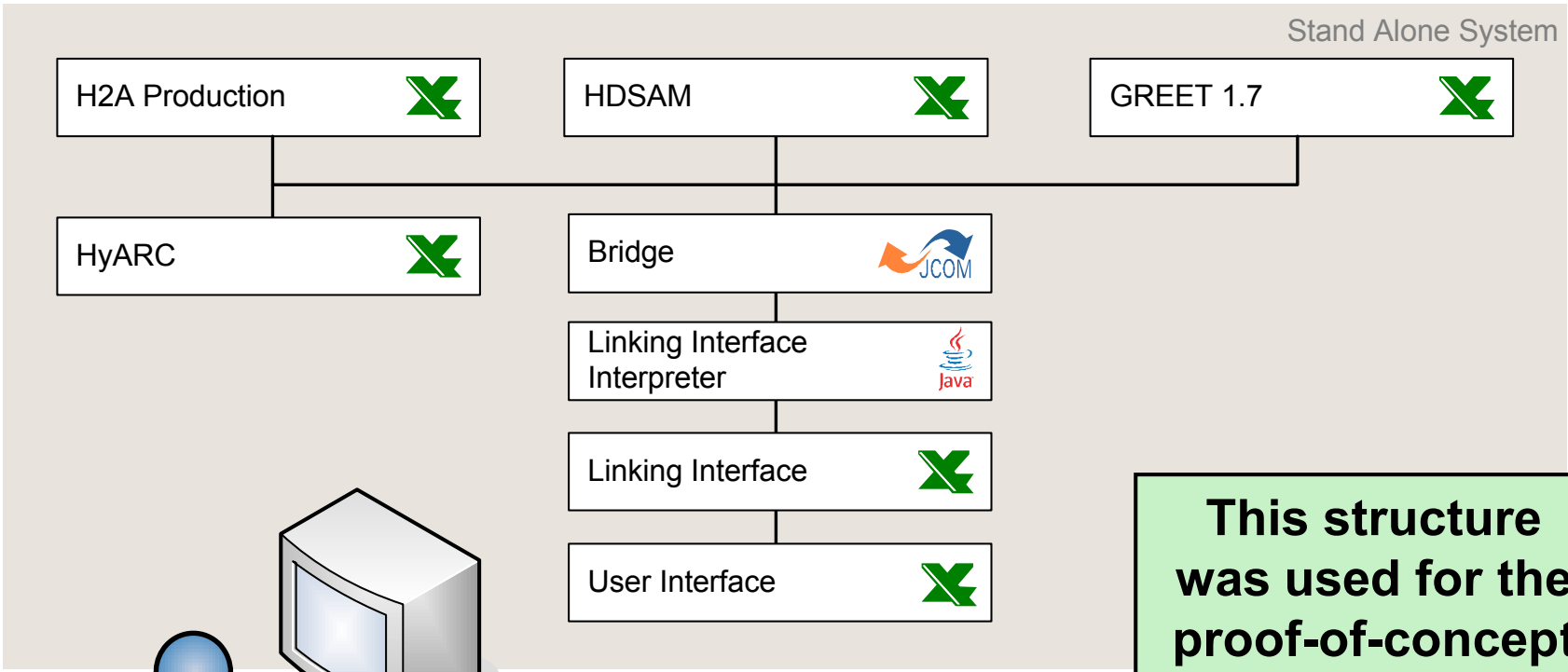
Comparison of hydrogen costs at the pump using different hydrogen production technologies.

How much hydrogen needs to be produced to supply a given city its demands?

What are the raw material needs to meet those demands?

Issues we are addressing initially

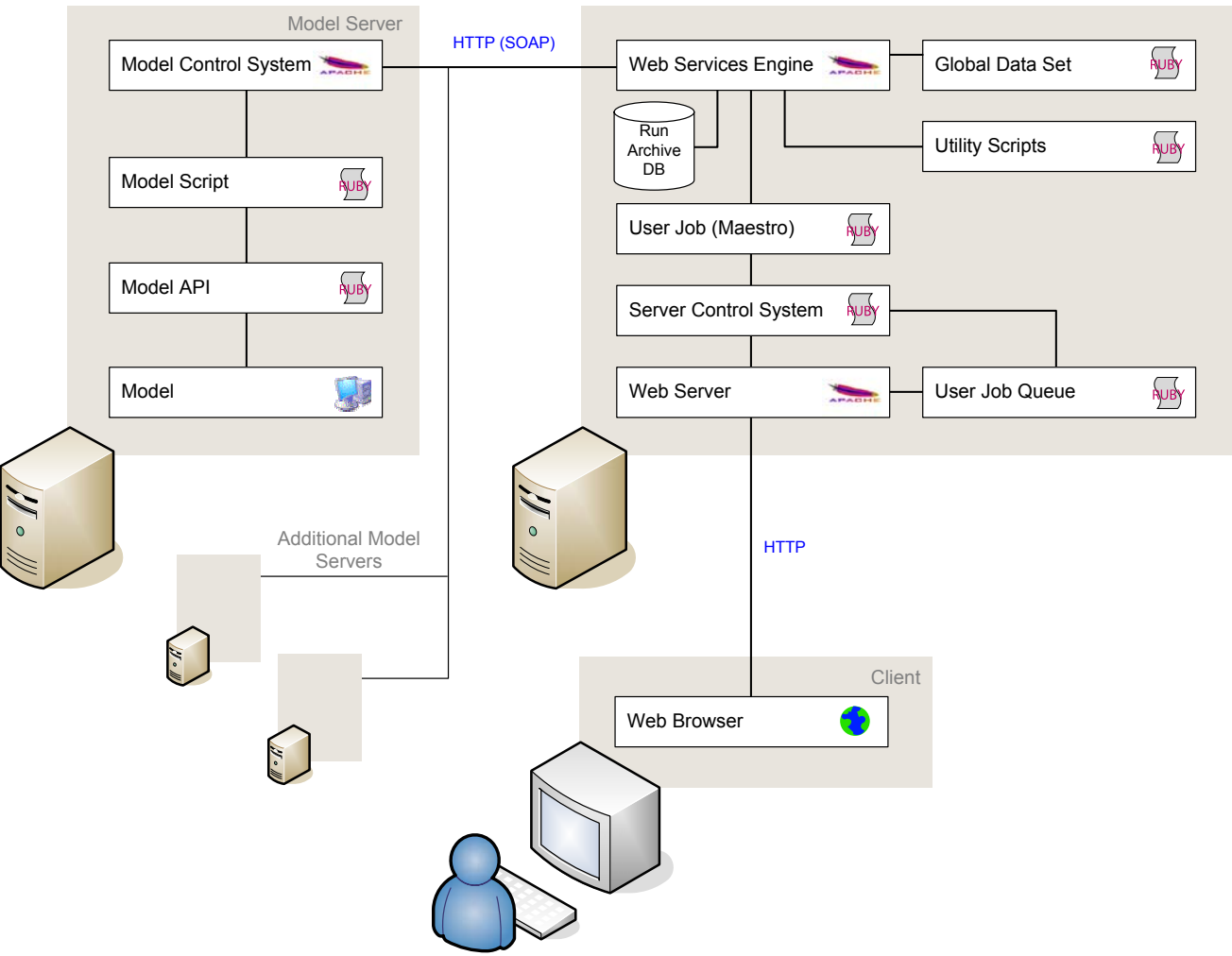
Earlier Work: Structure of Initial MSM



This structure was used for the proof-of-concept version of the MSM

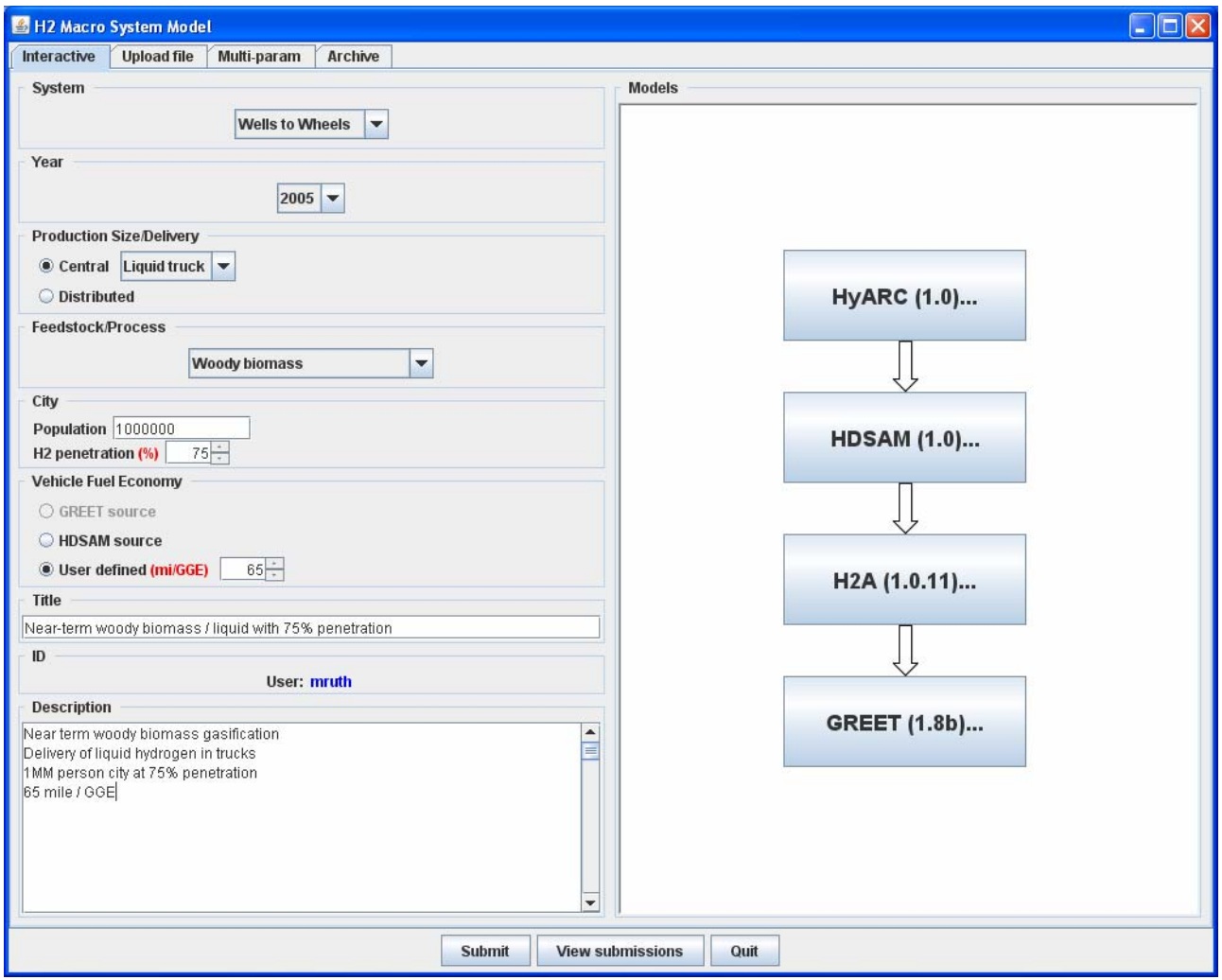
- **Federated Object Model (FOM) approach was selected**
- **Information to be transferred between models was identified**
- **An Excel-based linking interface was developed with a Java/COM application to transfer data between the linking spreadsheet**
- **Model use was validated & initial analysis completed**

Progress: Extensible/Robust Structure



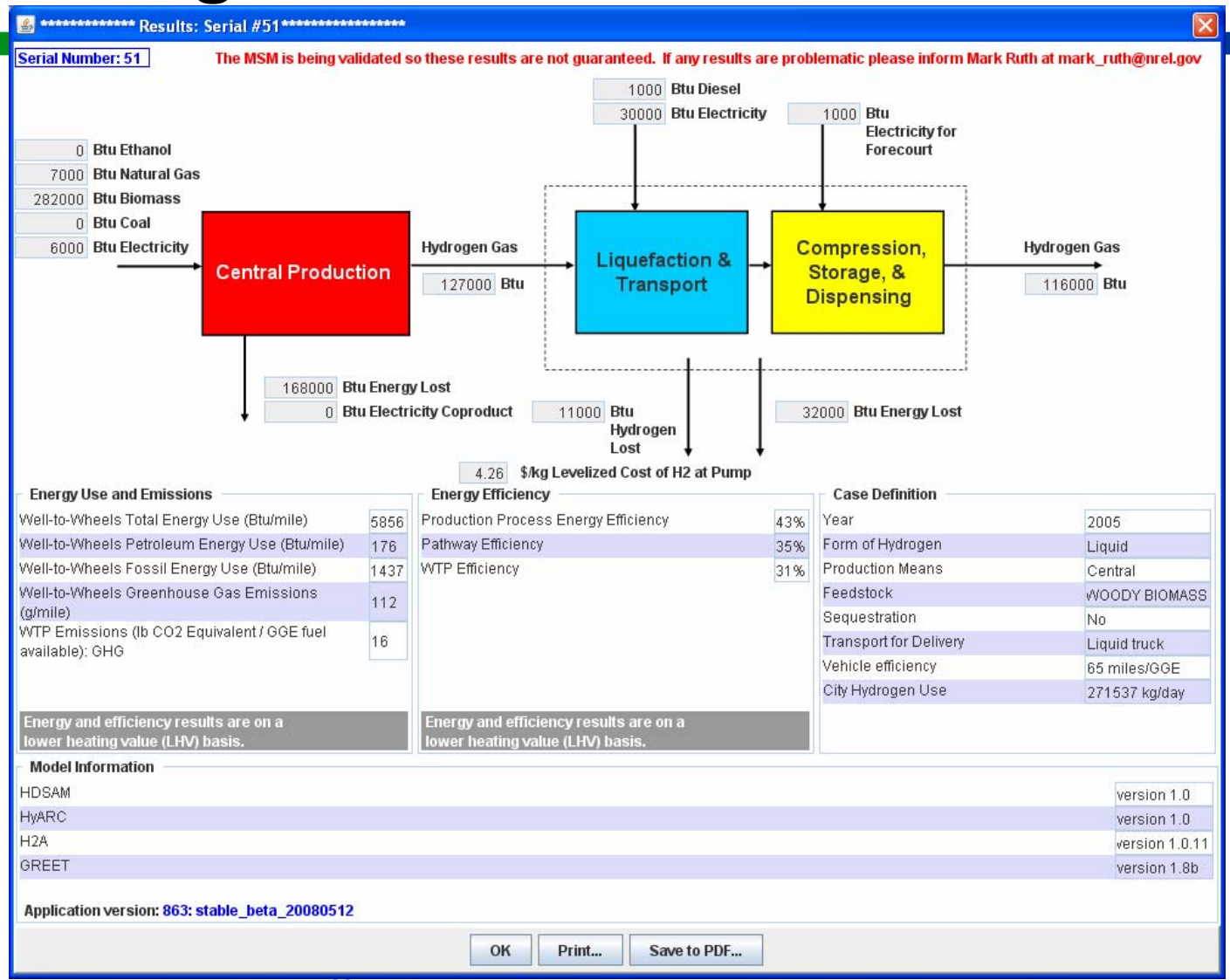
- Converted MSM structure from Excel/Java to Ruby
- Ruby version is more stable and allows for additional data types
- Developed technique that allows models to run on different machines
- Developed web-browser based graphical user interface (GUI) to make the MSM available to more users
- Validated results against proof-of-concept MSM

Progress: GUI & Web Interface



GUI available to hydrogen analysts at http://h2-msm.son.sandia.gov/
User defines technology, timeframe, population, and penetration.
MSM is run and model results generated.

Progress: GUI & Web Interface



Pathway costs, efficiencies, and well-to-wheels results are reported.

Pathway results are shown and user can print them or save them to a pdf.

User can also download the results in a csv file for table and figure creation.

Progress: Component Model Updates

Model	Proof-of-Concept MSM	Current MSM Version
HyARC	Heating values for hydrogen & fuels (downloaded in 2006)	Heating values for hydrogen & fuels (downloaded in 9/07)
H2A Production	Versions 1.0.9, 1.0.10, & 1.0.11 (downloaded in 2006)	Version 2.0 (Soon to be publicly available)
HDSAM	Version 1.0 (downloaded in 2006 & made a couple minor corrections)	Version 2.0 (Soon to be publicly available)
GREET	Version 1.7 (downloaded 2/21/07 & made a couple minor corrections)	Version 1.8B (downloaded 3/17/08 & made one minor correction)

Version updates required identification of modified input and output cells, modified model structure, and validation of results from the new model.

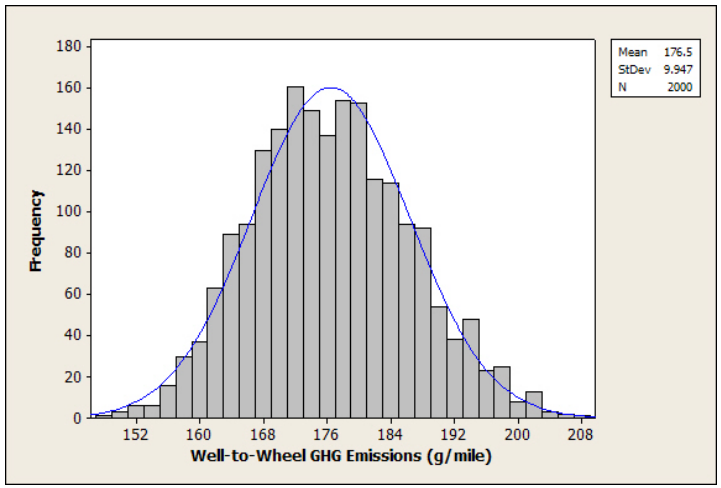
Green fill indicates model versions used for results on previous slide

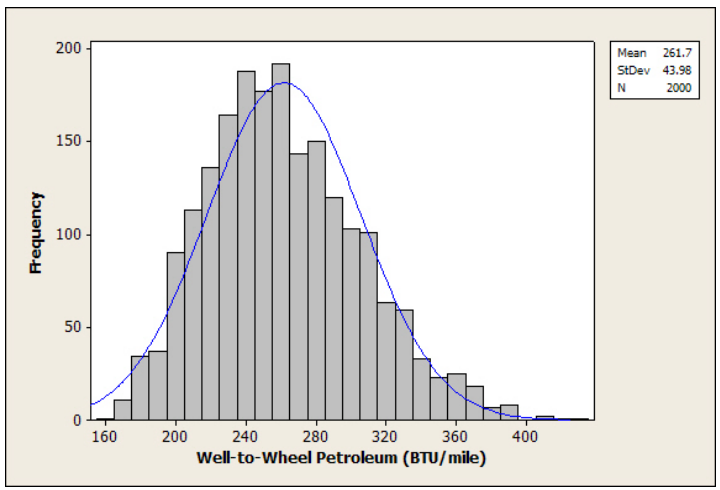
Progress: Stochastic Capability

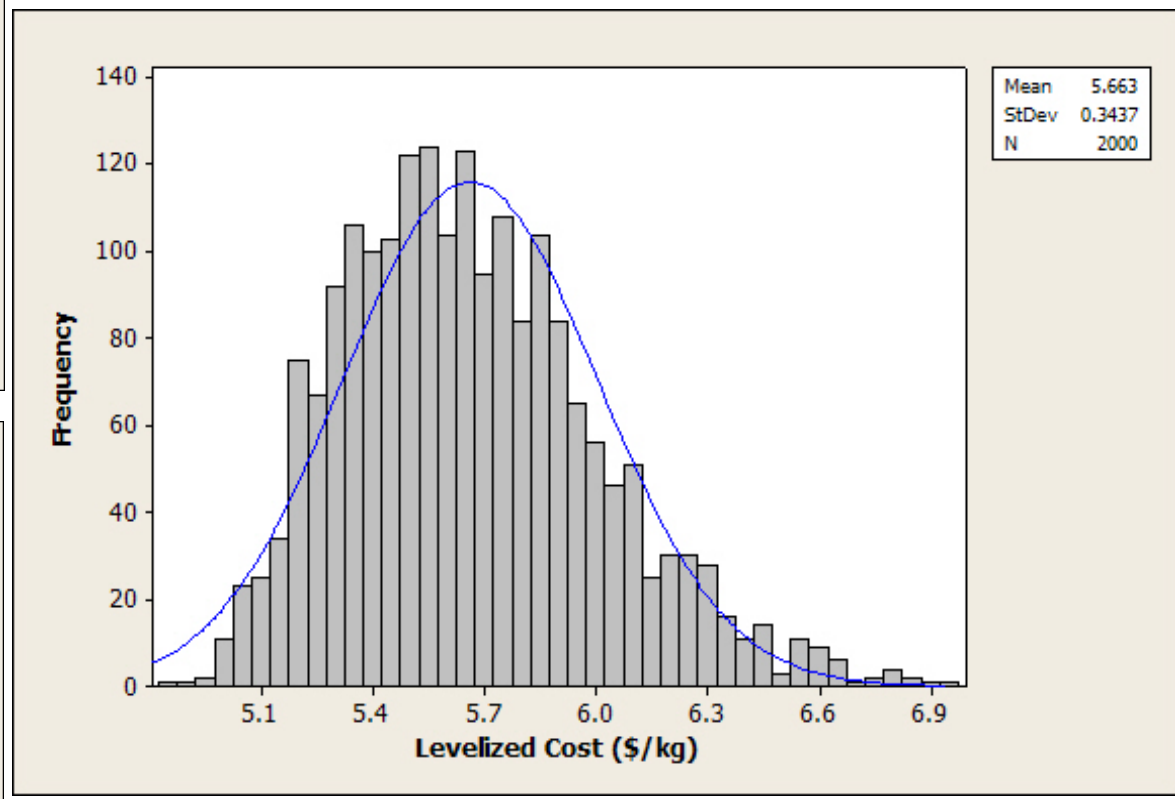
- **Monte Carlo simulation using DAKOTA (http://www.cs.sandia.gov/DAKOTA/)**
  - **DAKOTA (Design Analysis Kit for Optimization and Terascale Applications) toolkit was developed at Sandia**
  - **It provides algorithms for optimization; uncertainty quantification; parameter estimation; and sensitivity/variance analysis.**
- **Example Analysis**
  - **Near term biomass gasification with liquid hydrogen delivery in trucks to a 250,000 person city with 50% penetration**
  - **# samples = 2000**
  - **7 inputs, triangular distribution**
    - **Biomass feedstock consumption (kg/kg_H2)**
    - **Biomass feedstock cost (dollar/kg)**
    - **Vehicle fuel efficiency (mile/GGE)**
    - **Production FTEs**
    - **Production total capital investment (dollar)**
    - **Production capacity factor**
    - **Poplar farming energy use (joule/kg)**
  - **5 outputs/responses**
    - **Well-to-Wheel total energy consumption (Btu/mile)**
    - **Well-to-Wheel fossil fuels consumption (Btu/mile)**
    - **Well-to-Wheel GHG emissions (g/mile)**
    - **Well-to-Wheel petroleum energy consumption (Btu/mile)**
    - **Pathway levelized cost (dollar/kg)**

Progress: Stochastic Capability

Example Results







Analysis run with H2A V 1.0.9, HDSAM V 1.0, and GREET 1.7

Progress: Documentation

- Draft user manual available
- Provides an overview
  - Goals
  - Scope
  - Component model links
  - Model structure
  - Restrictions, assumptions, constraints
- Provides guidance
  - Typical end user (using web-based GUI)
  - Advanced user (using Ruby and own versions of models)
- Is a living document that will be updated as the MSM is modified.

Progress: Validating Use of Models

Discussions with Model Developers
- Understand the model's purpose & use
- Compile lists of inputs and results
- Recommend modifications to component models

Understand models intimately
- Definition of terms
- Calculation methodology

Comparison to other analyses & previous MSM runs
- Meticulous review of inputs & results
- Mapping between results from different analyses
- Many pathways were mapped to the posture plan
- Other pathways were compared in the HyWAYS / IPHE project

Interaction with community (analysts & industry)
- Present & discuss methods & results
- Reach consensus on approach & parameters

Key Assumptions

Pathway assumptions are entered. Other assumptions are embedded in the models being linked but are changed in sensitivity runs

Pathway Assumptions

- Full-deployment scenario
- Urban demand area
- 250,000 person city
- 50% H_2 penetration
- 1500 kg/day stations
- Mid-size FCV –
  - Current - 57.1 mi / GGE
  - Advanced – 62.7 mi / GGE

Financial

- 10% DCFROR
- 20 year plant life
- MACRS depreciation where appropriate

Production

- Central Biomass
  - Current – 45% conversion eff.
  - Advanced – 51% conversion eff.
- Coal Gasification
  - Current – 72% gasifier eff. & 80% PSA eff.
  - Advanced – 72% gasifier eff. & 95% HSD eff.
- Central Natural Gas Reforming
  - Current – 82% SMR eff. & 80% PSA eff.
  - Advanced – 82% SMR eff. & 80% PSA eff.
- Distributed SMR
  - Current – 68.7% production unit efficiency
  - Advanced – 83.7% production unit efficiency
- Distributed Electrolysis
  - Current – 64% production efficiency
  - Advanced – 67% production efficiency

HDSAM

- Fueling station capacity factor = 0.7
- 62 miles from central production to city
- Liquefier efficiency 75.5%

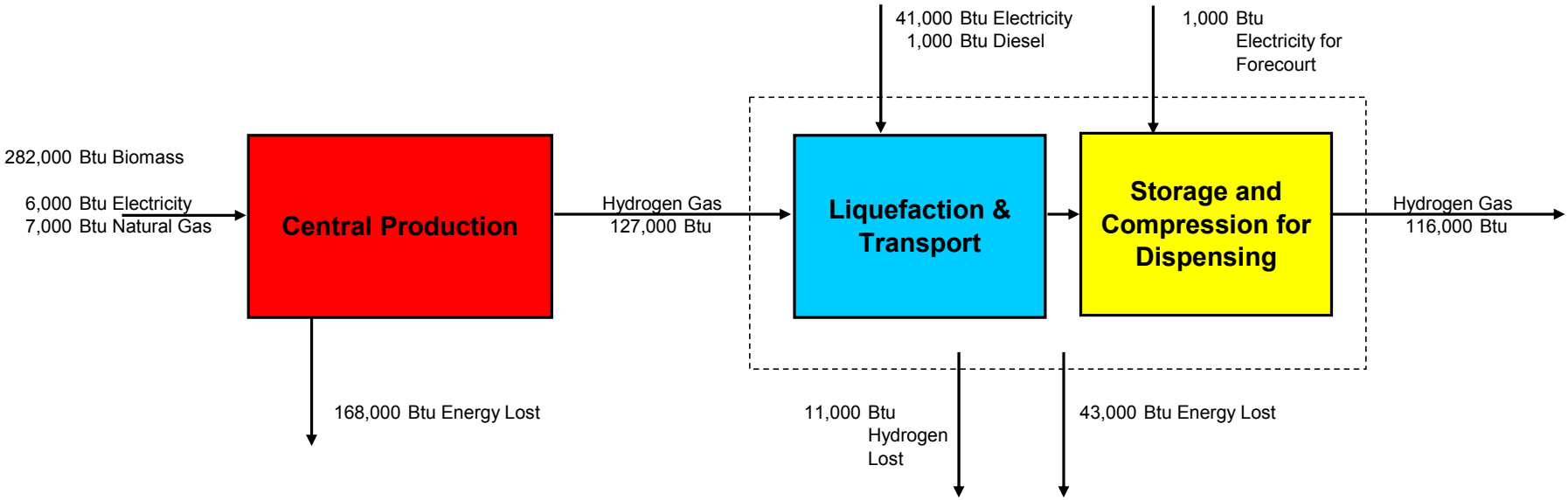
GREET

- Gasoline is RFG without oxygenate
- Current technologies use US average grid mix
- Advanced technologies use future grid mix with 85% of CO_2 from coal plants sequestered

Analysis: Posture Plan Comparison

Reviewed all pathways in 2006 Hydrogen Posture Plan

Near-term biomass liquid pathway MSM results shown in black
Posture plan results shown in blue



Well-to-Wheels Total Energy Use (Btu/mile)	7,426	6600
Well-to-Wheels Petroleum Energy Use (Btu/mile)	235	200
Well-to-Wheels Greenhouse Gas Emissions (g/mile)	180	190
Levelized Cost of H2 at Pump ($/kg)	5.43	5.10

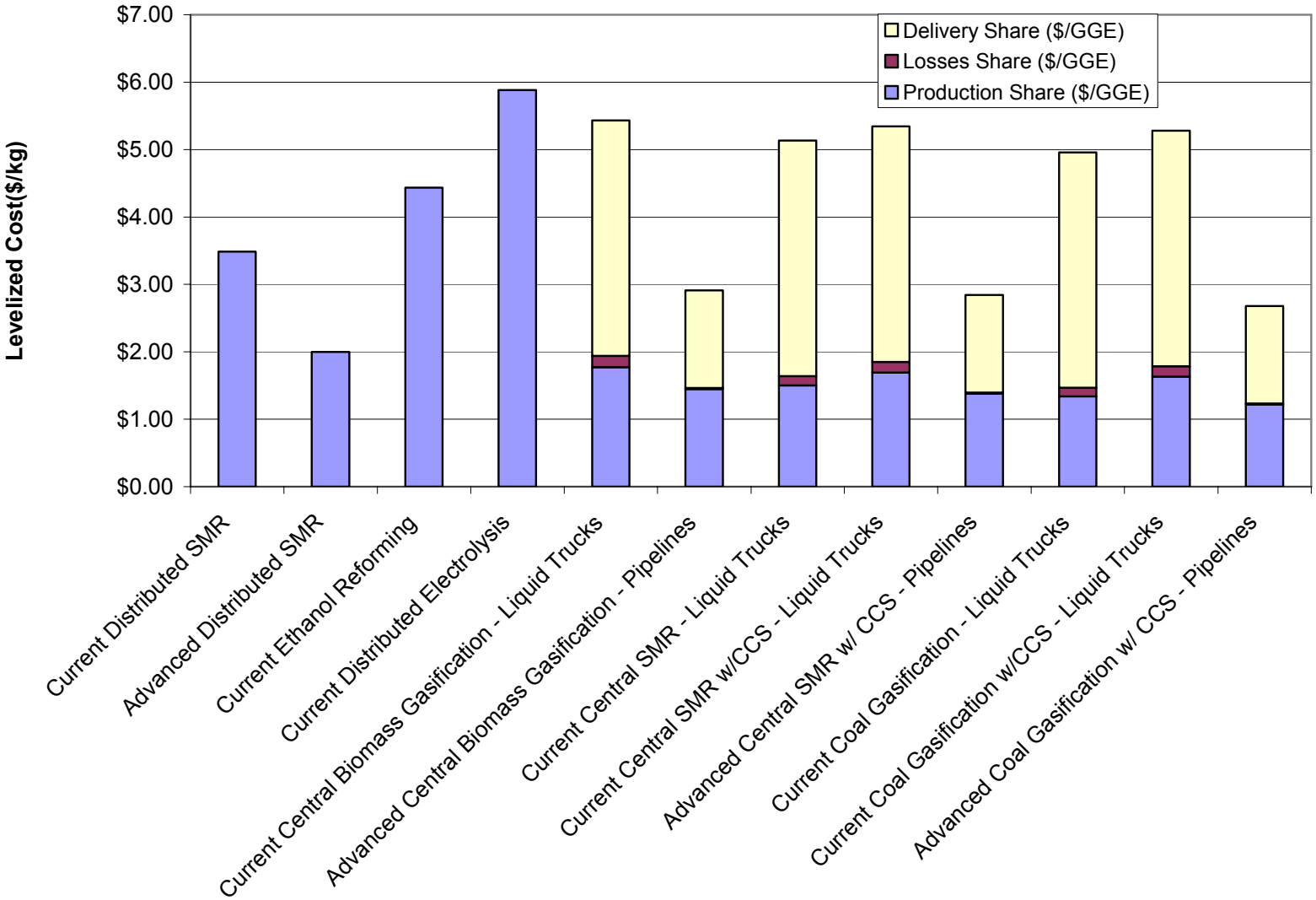
Production Process Energy Efficiency	43%	45%
Pathway Efficiency	34%	40%

Case Definition
Year: 2005
Hydrogen as Liquid
Central Production

- **Hydrogen losses were not fully incorporated in the posture plan. Incorporation of those losses drove up energy use and emissions.**
- **In the posture plan, GREET was set to herbaceous biomass. Setting GREET to use woody biomass reduced GHG emissions.**
- **The production and liquefaction efficiency were slightly different between HDSAM & GREET. Making them consistent affected results.**

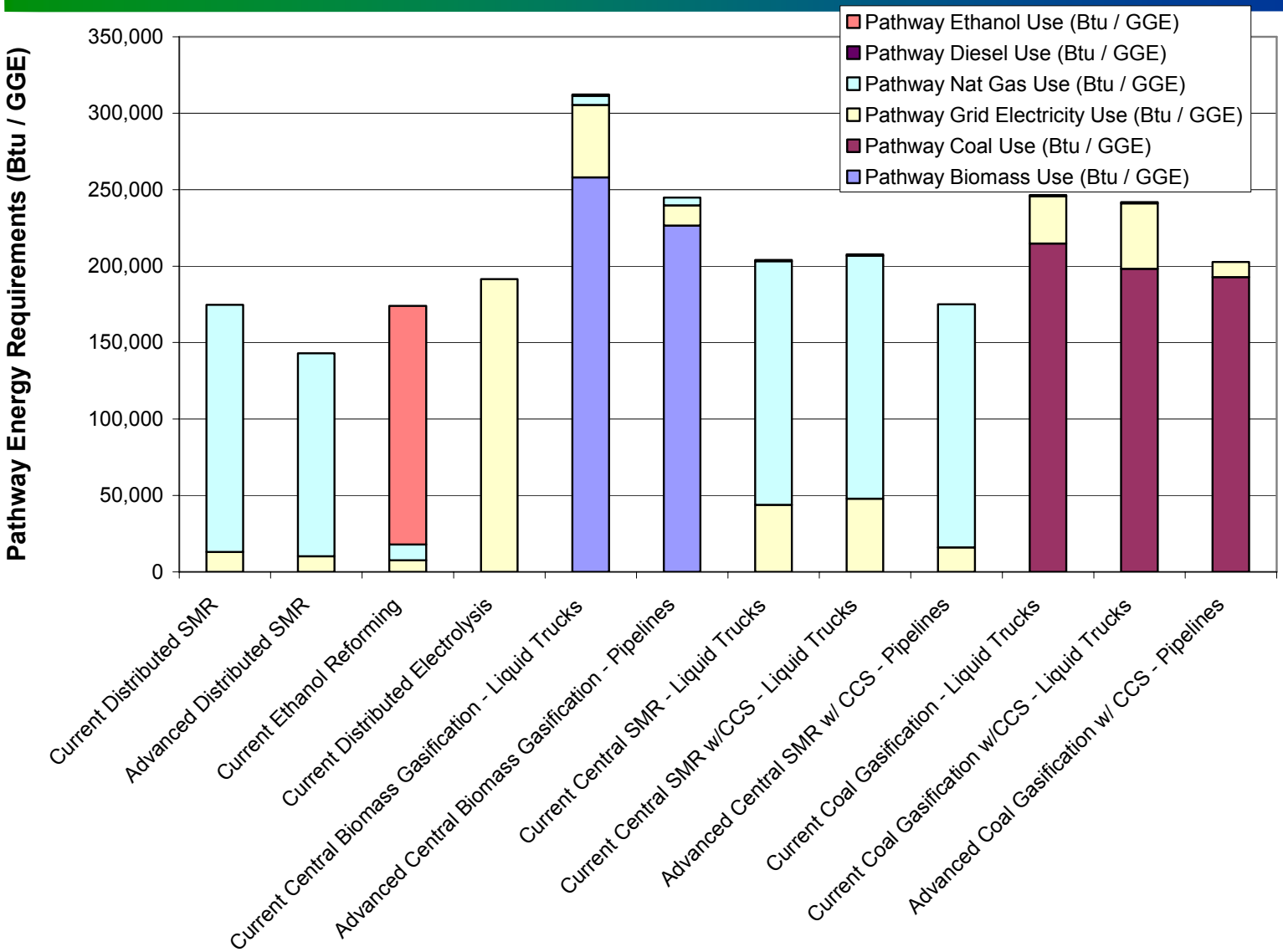
Case R070903F

Analysis: Comparison of Levelized Costs



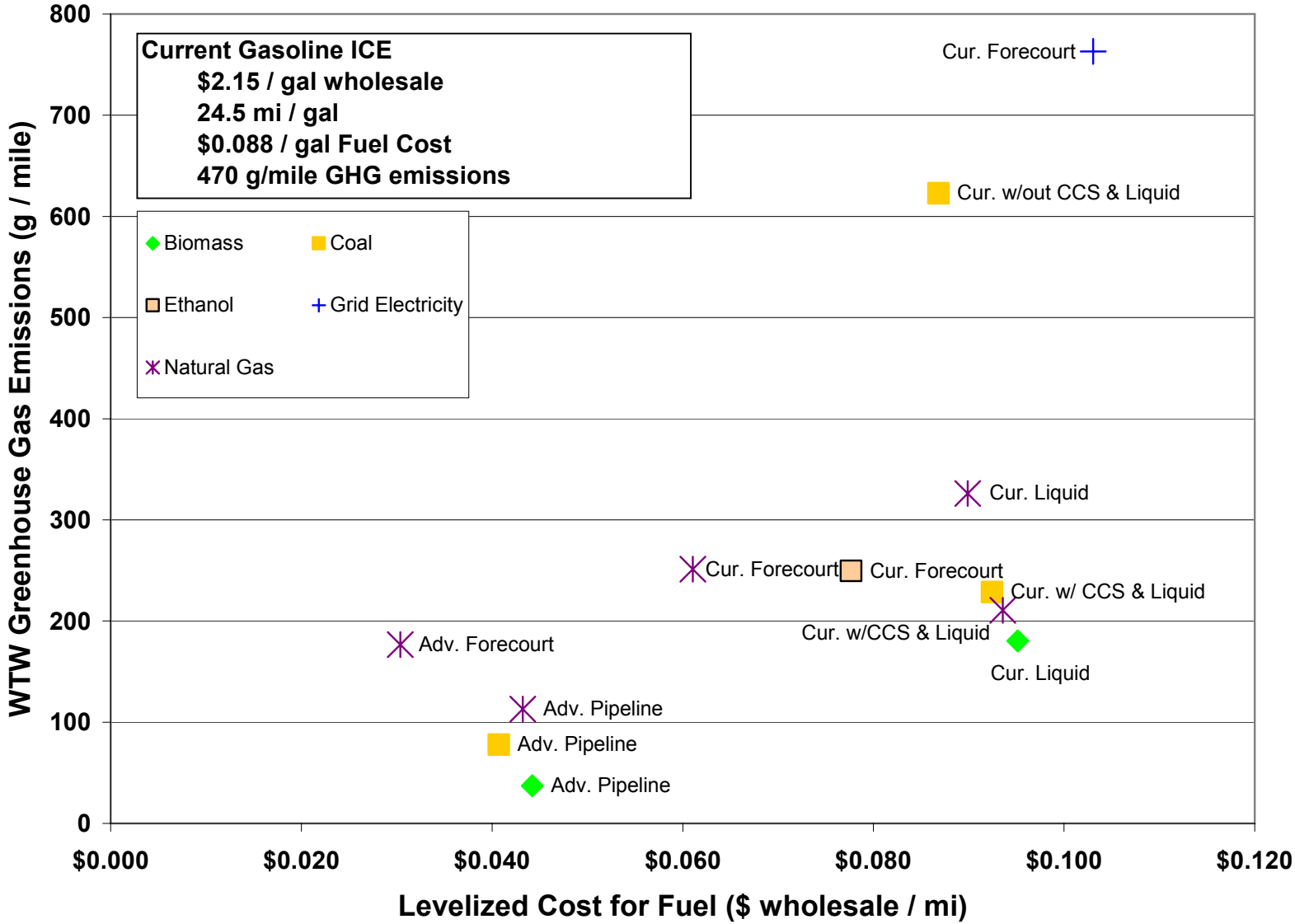
Results from proof-of-concept version of the MSM

Analysis: Comparison of Energy Use



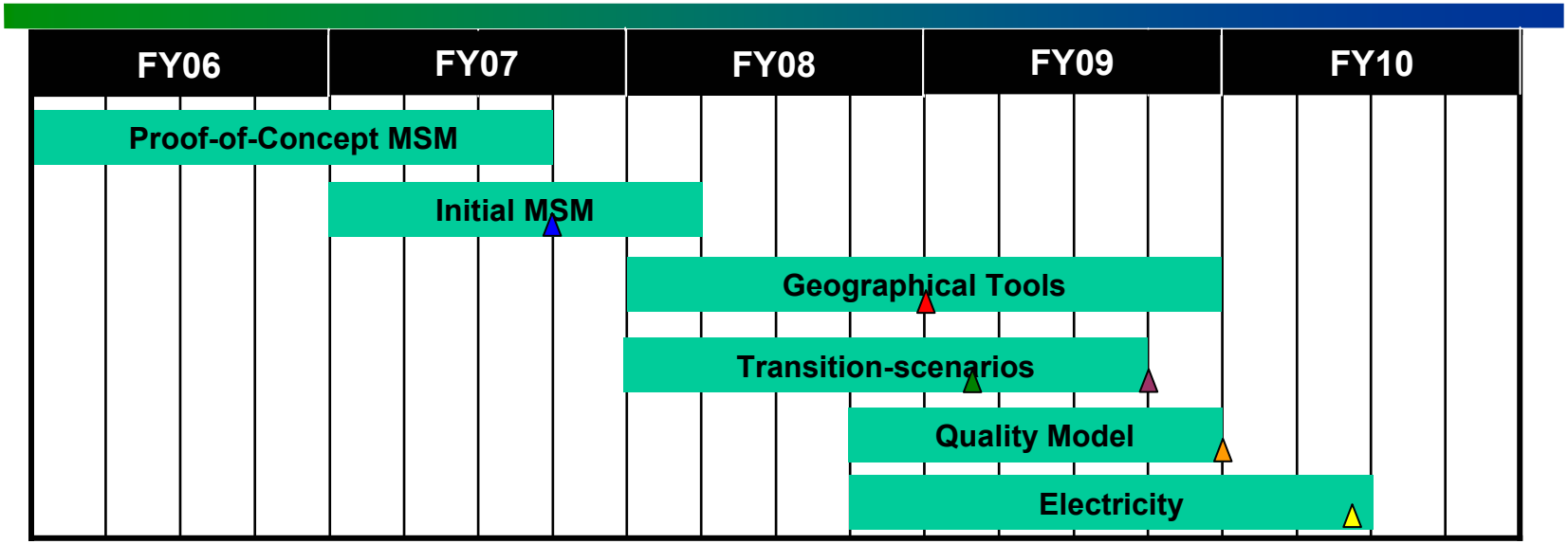
Results from proof-of-concept version of the MSM

GHG Emissions vs Fuel Cost



Results from proof-of-concept version of the MSM

Proposed Future Work



- Proof-of-Concept MSM (H2A Production, HDSAM, GREET linked with Excel and Java)
  - Peer-reviewed (September 11, 2007)
- Initial version of an extensible MSM (H2A Prod., HDSAM, GREET linked with Ruby)
  - Create a stable, extensible, and user-friendly MSM
  - ▲ Make MSM available on password protected internet site (September 11, 2007)
  - Develop stochastic modeling capability and decision-making tools
- Link geographical tools to MSM
  - ▲ Initial linkage of HyDRA to the MSM (September 30, 2008)
  - Full linkage of HyDRA to the MSM
- Link transition-scenario models to MSM
  - Determine next set of issues that need to be addressed
  - ▲ Link HyPRO to MSM (November 30, 2008)
  - Consider linking HyTRANS or HyDS
  - ▲ Review transition scenarios using the MSM (June 30, 2009)
- ▲ Link hydrogen quality model to MSM (September 30, 2009)
- ▲ Add stationary electrical generation and electrical infrastructure (February 28, 2010)

DOE Hydrogen Program

Summary

- The MSM is being built to address priority analysis issues
- The proof-of-concept version of the MSM includes H2A Production, HDSAM, and GREET . It was used for analysis and has been updated.
- A web-based MSM GUI is available to hydrogen analysts.
- Stochastic capability has been added to the MSM
- The MSM is being used for programmatic analysis.

Acknowledgements

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