DOE Hydrogen Program

Macro-System Model

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Project ID # AN5

Overview

Timeline

- Start date: Feb 2005
- Completion: Sept 2010
- Percent complete: 20%

Budget

- Total funding:
  - 100% DOE funded
- FY06 funding:
  - $184K NREL/SIO
  - $280K Sandia NL
  - $60K other national lab work
- FY07 funding
  - $190K NREL/SIO
  - $336K Sandia NL

Barriers

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

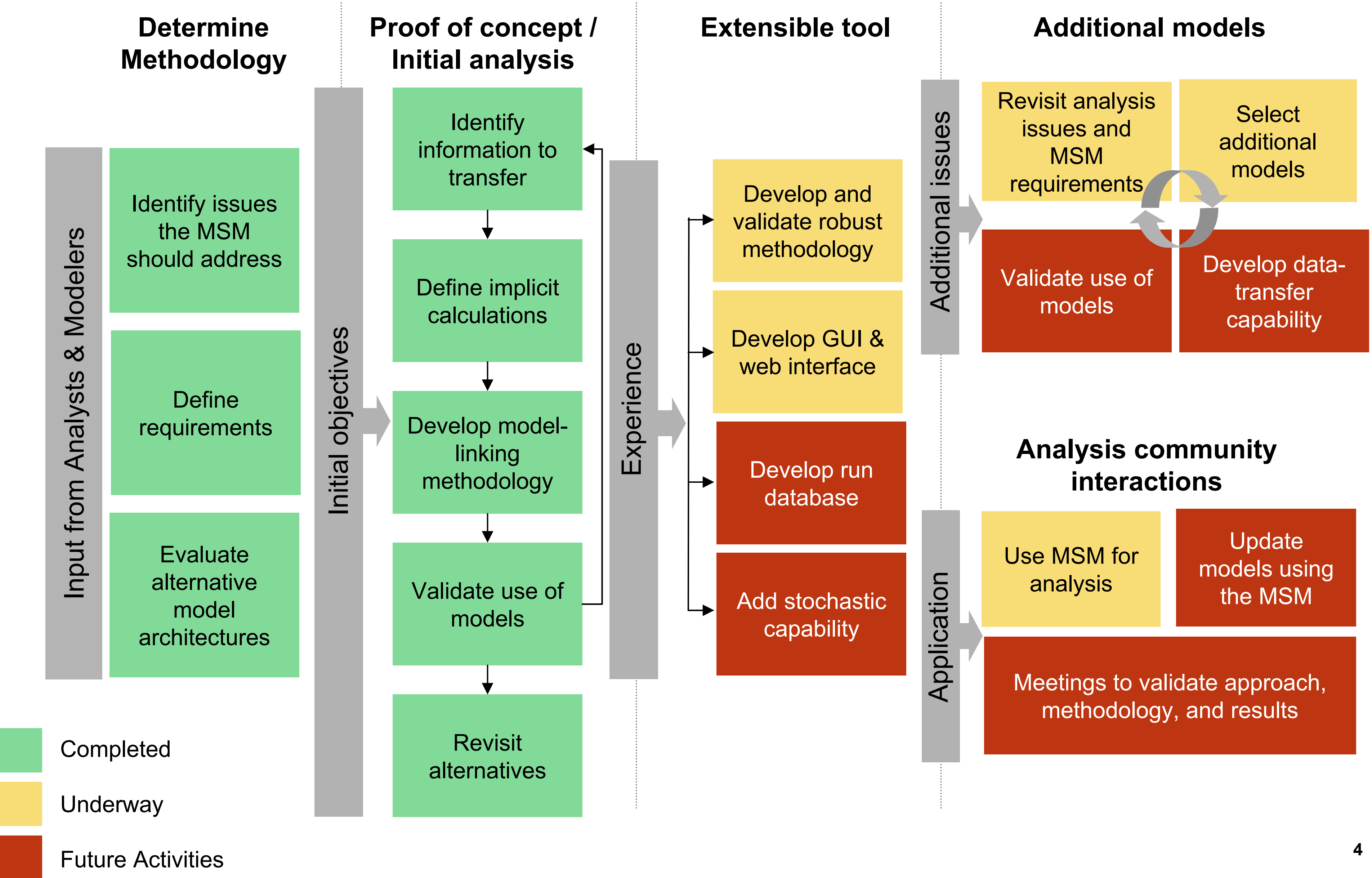
Partners

- Sandia National Laboratory (computational development)
- NREL (H2A Production, well-to-wheel analysis validation, HyDRA)
- ANL (HDSAM, GREET, well-to-wheel analysis validation)
- 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
- **2006/2007 objectives**
  - Include additional hydrogen pathway technologies
  - Validate use of models in pathways
  - Comparative and trade-off analyses
  - Revisit alternatives for the MSM methodology
  - Begin development of robust MSM methodology that can accommodate multiple users

Approach: MSM Development



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Progress: 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?

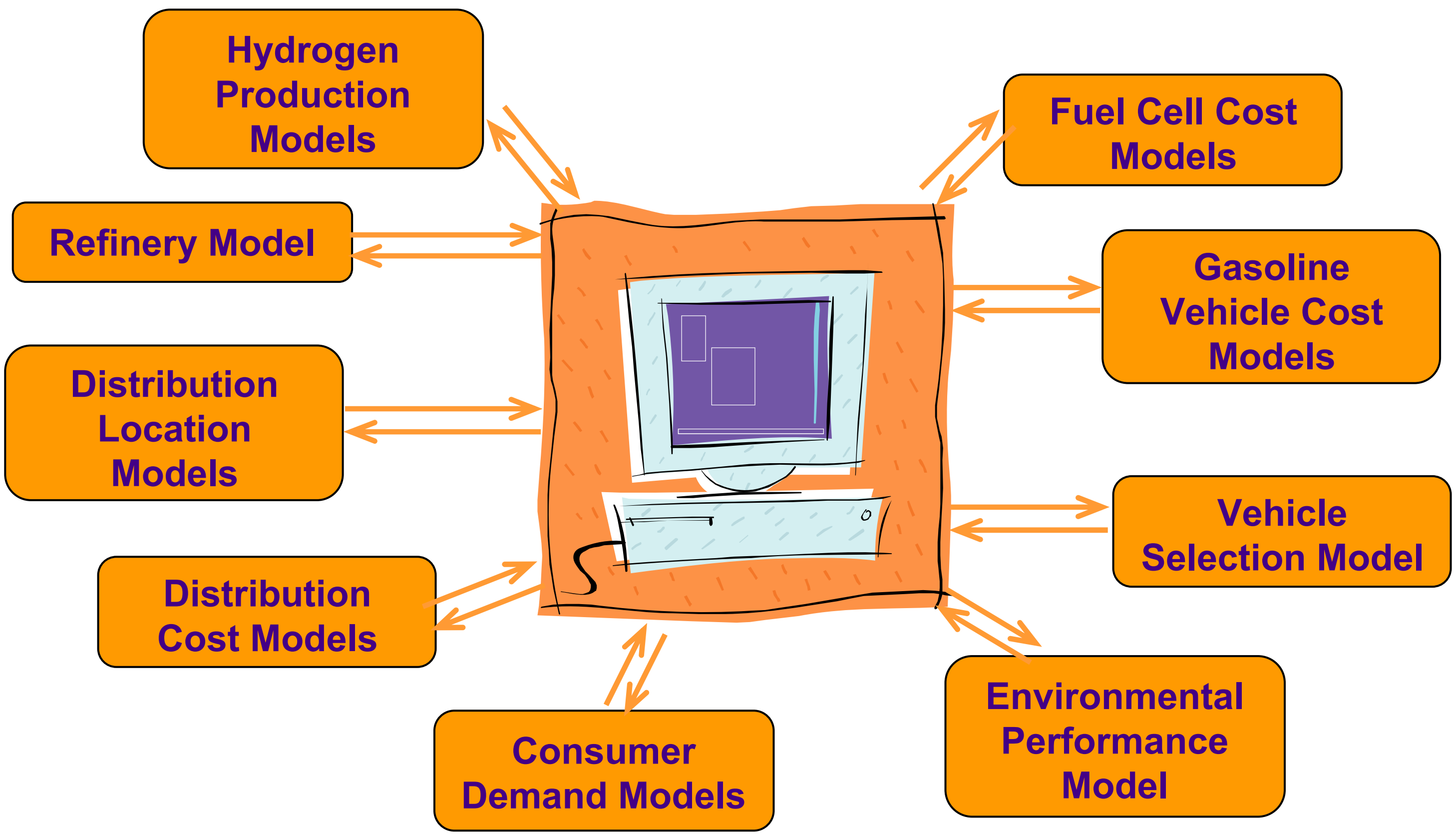
What are the raw material needs to meet those demands?

Issues we are addressing initially

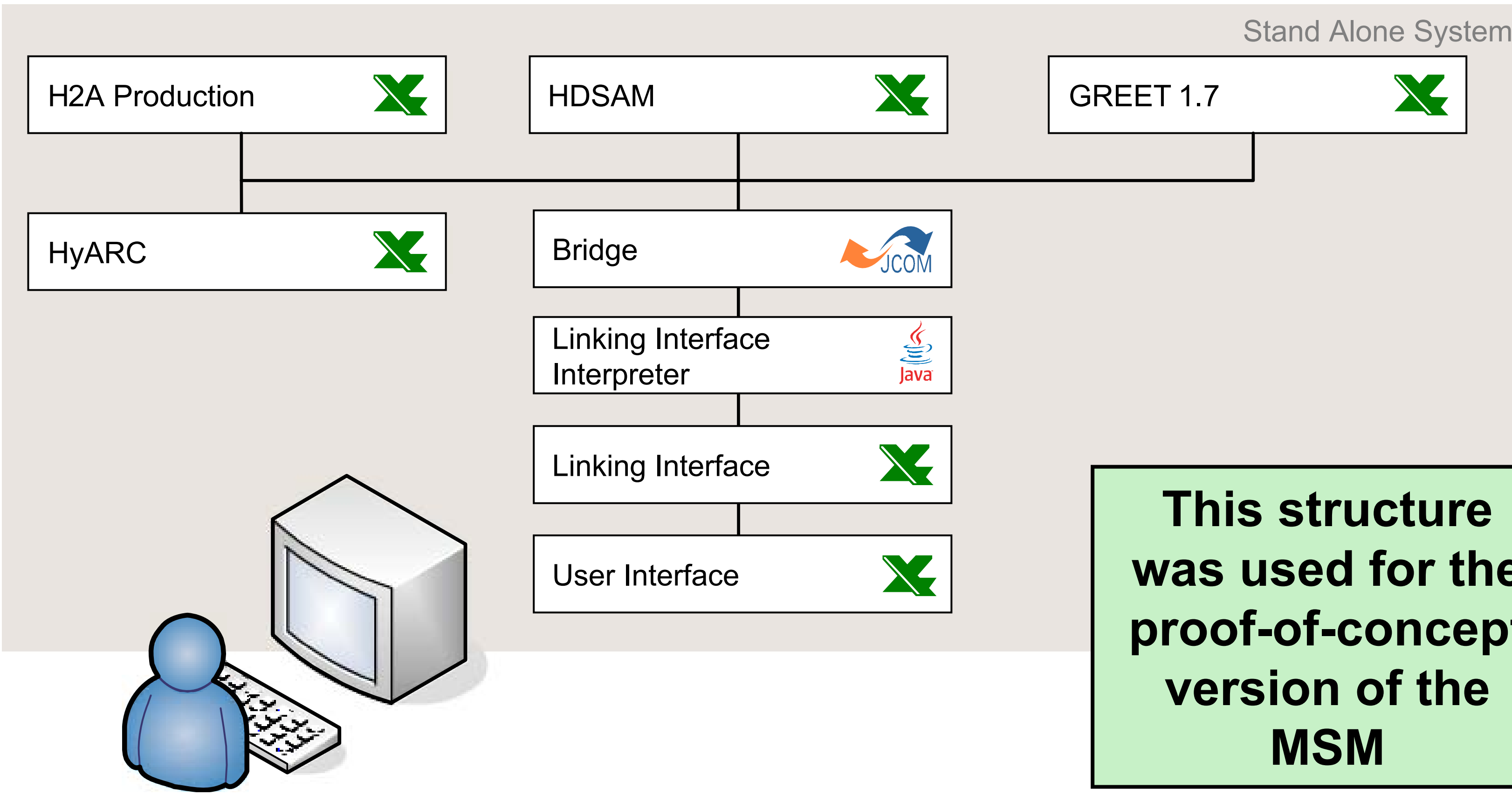
Progress: Selected MSM Approach

Federated Object Model (FOM) – capable of integrating and utilizing existing and emerging component models (federates)

A single interface is used to share inputs, credible / documented data, and outputs between models



Progress: Structure of Initial MSM



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

- **Information to be transferred between models has been identified**
- **An Excel-based linking interface has been developed**
- **Sandia developed a Java/COM application to transfer data between the linking spreadsheet and the models and launch macros when appropriate**
- **Model use has been validated**

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Progress: Pathways in MSM

Technology Timeframe	Location	Production Technology	Carbon Sequestration	Delivery Technology
Current	Central	Biomass Gasification	None	Trucks With Liquid
Current	Central	Coal Gasification	90%	
Current	Central	Coal Gasification	None	
Current	Central	NG Reforming	73%	
Current	Central	NG Reforming	None	
Current	Central	Biomass Gasification	None	Pipelines Carrying Gas
Current	Central	Coal Gasification	90%	
Current	Central	Coal Gasification	None	
Current	Central	NG Reforming	73%	
Current	Central	NG Reforming	None	
Current	Forecourt	Electrolysis	None	None
Current	Forecourt	NG Reforming	None	
Advanced	Central	Biomass Gasification	None	Trucks with Liquid and Pipelines Carrying Gas
Advanced	Central	Coal Gasification	90%	
Advanced	Central	NG Reforming	73%	
Advanced	Central	NG Reforming	None	
Advanced	Forecourt	Electrolysis	None	None
Advanced	Forecourt	NG Reforming	None	

Pathways in green were available before the 2006 AMR but had not been validated.
The remainder were added during this year.
Model interactions for all pathways were validated this year.

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

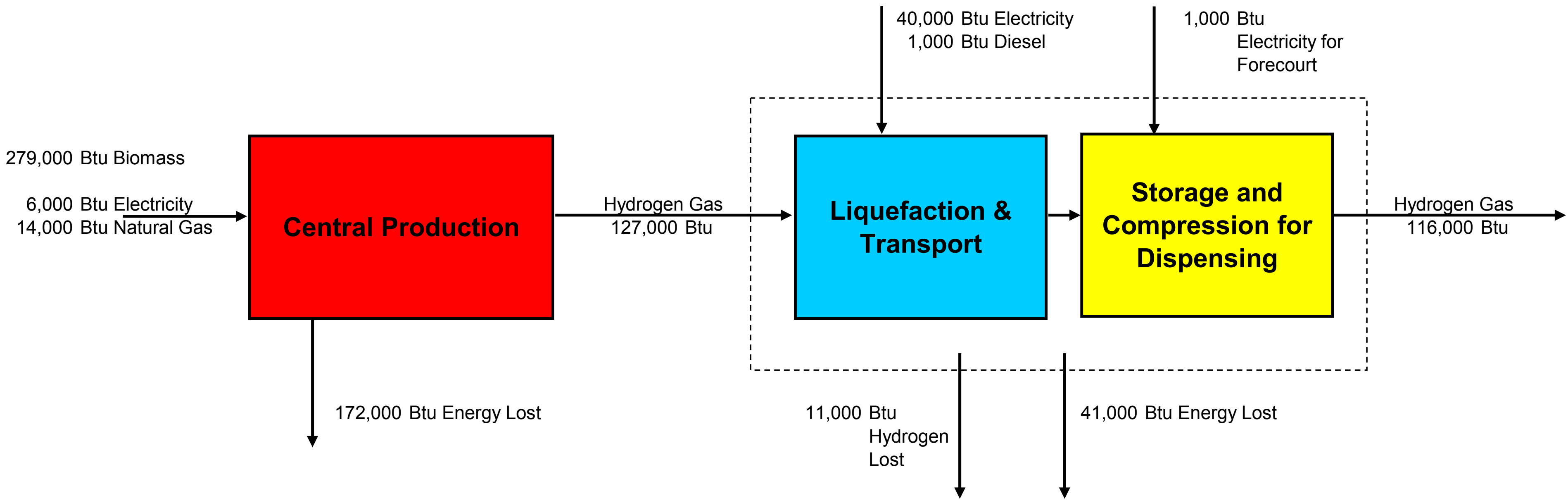
Production
- Central Biomass
  - Current – 45% conversion eff.
  - Advanced – 51% conversion eff.
- Coal Gasification
  - Current – 72% gasifier eff. & 80% PSA eff.
  - Advanced – 72% gasifier eff. & 95% HSD eff.
- Central Natural Gas Reforming
  - Current – 82% SMR eff. & 80% PSA eff.
  - Advanced – 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

Pathway Results

Current Biomass Gasification with Liquid Hydrogen Delivered in Trucks



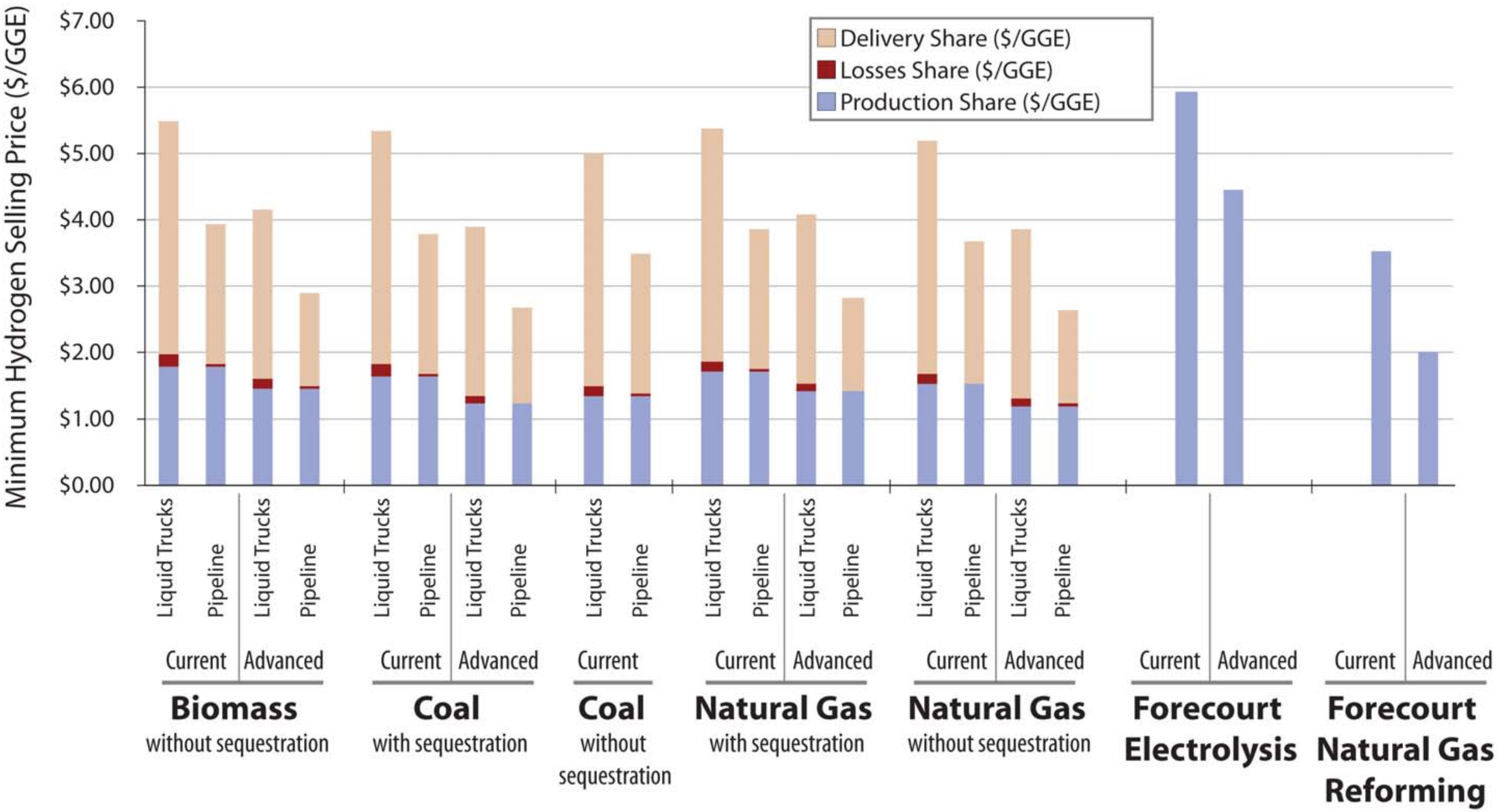
Well-to-Wheels Total Energy Use (Btu/mile)	7,342
Well-to-Wheels Petroleum Energy Use (Btu/mile)	232
Well-to-Wheels Greenhouse Gas Emissions (g/mile)	179
Levelized Cost of H2 at Pump ($/kg)	5.47

Production Process Energy Efficiency	44%
Pathway Efficiency	35%
WTP Efficiency	28%
WTP Emissions (lb CO2 Equivalent / GGE fuel available):	22

Case Definition
Year: 2005
Hydrogen as Liquid
Central Production
Woody Biomass Feedstock
Sequestration: No
Transport for Delivery: Truck
Vehicle Efficiency: 57.1 mile / GGE
City Hydrogen Use: 51517 kg/day

Case R070424F

Levelized Cost Results

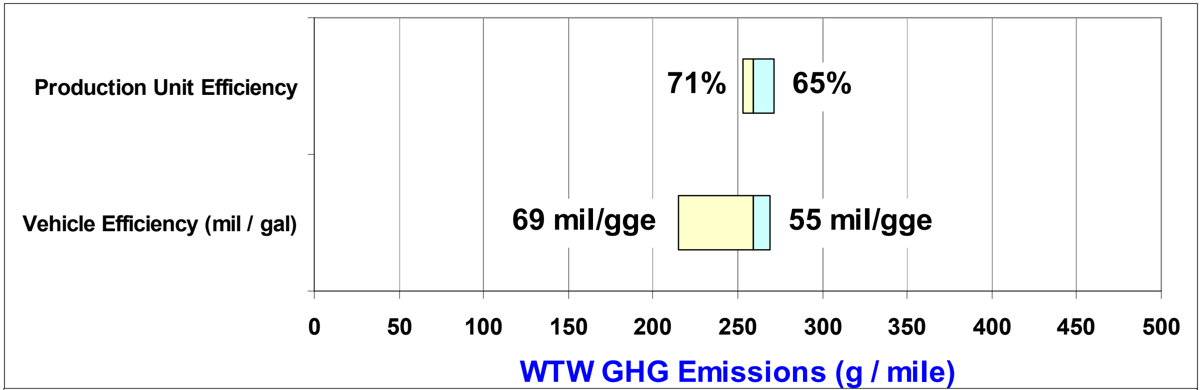


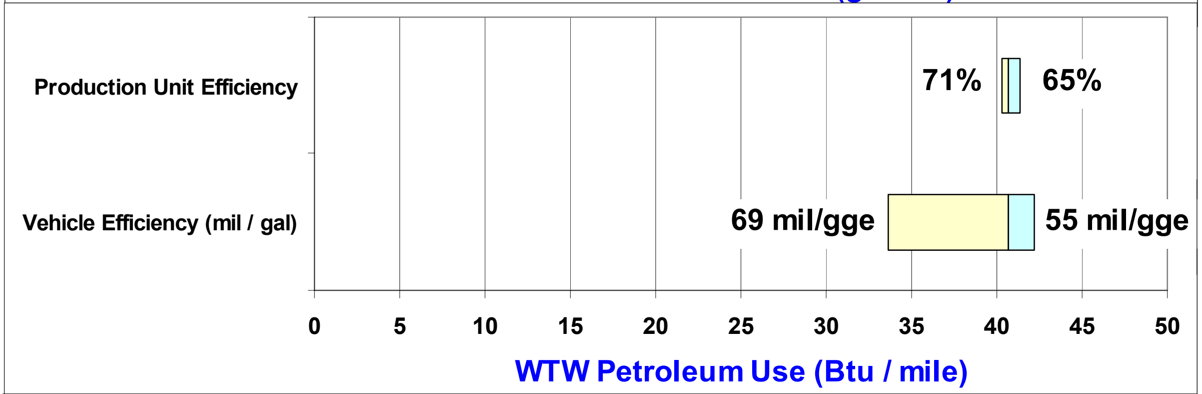
The MSM eases comparisons of levelized cost at the pump

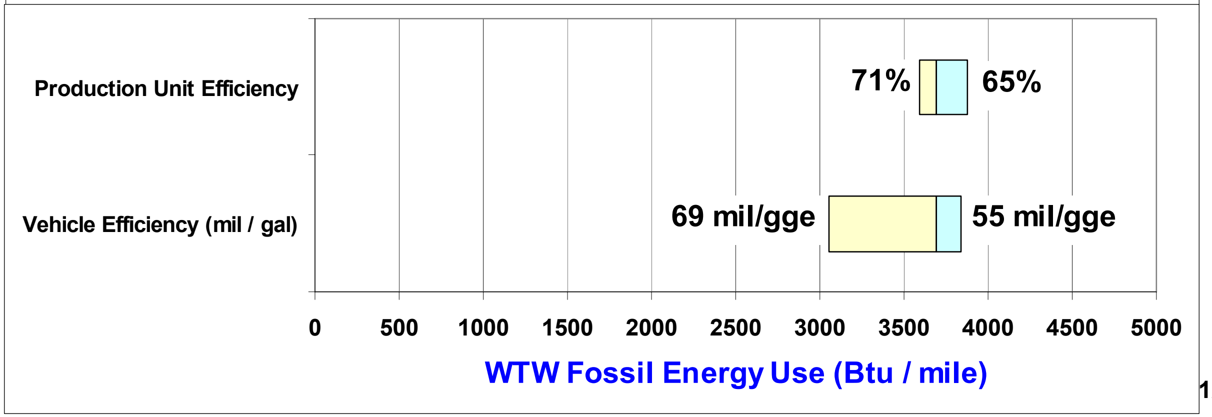
Sensitivity Results

Distributed SMR Production Efficiency vs. Vehicular Efficiency

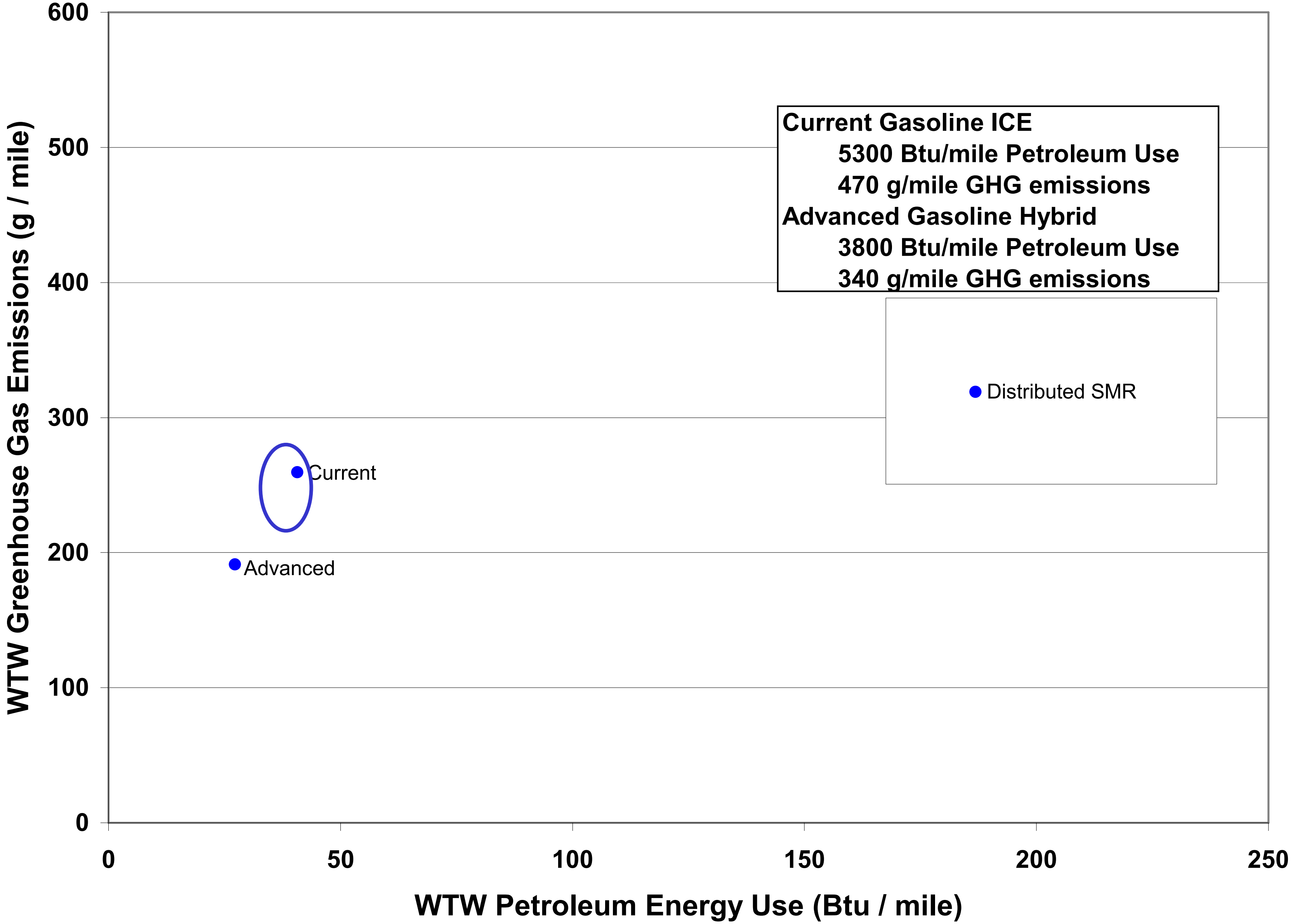
- Current Technology
- Base production unit efficiency is 68.7%
- Base vehicular efficiency is 57.1 mile / GGE







Petroleum Use vs GHG Emissions



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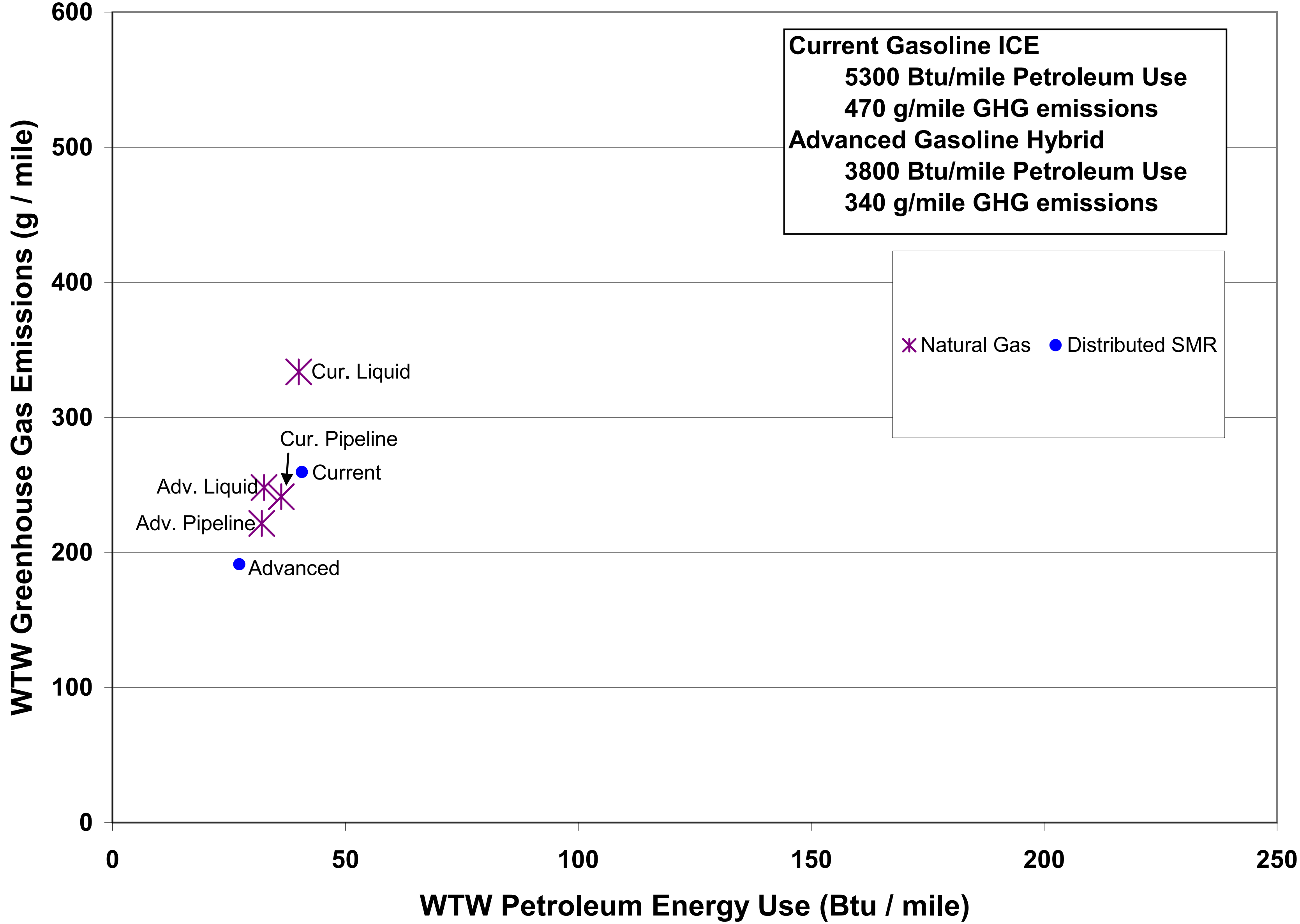

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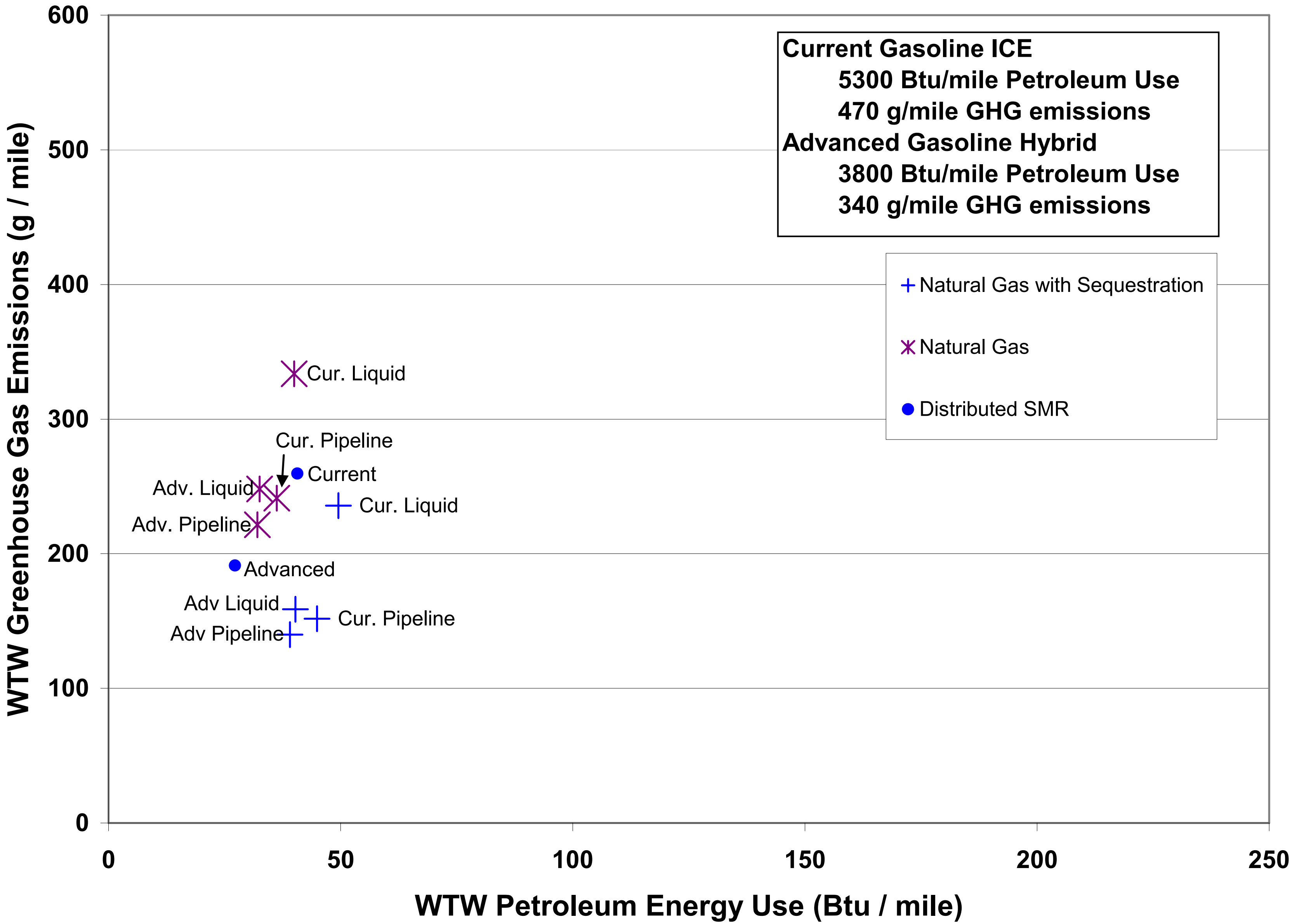

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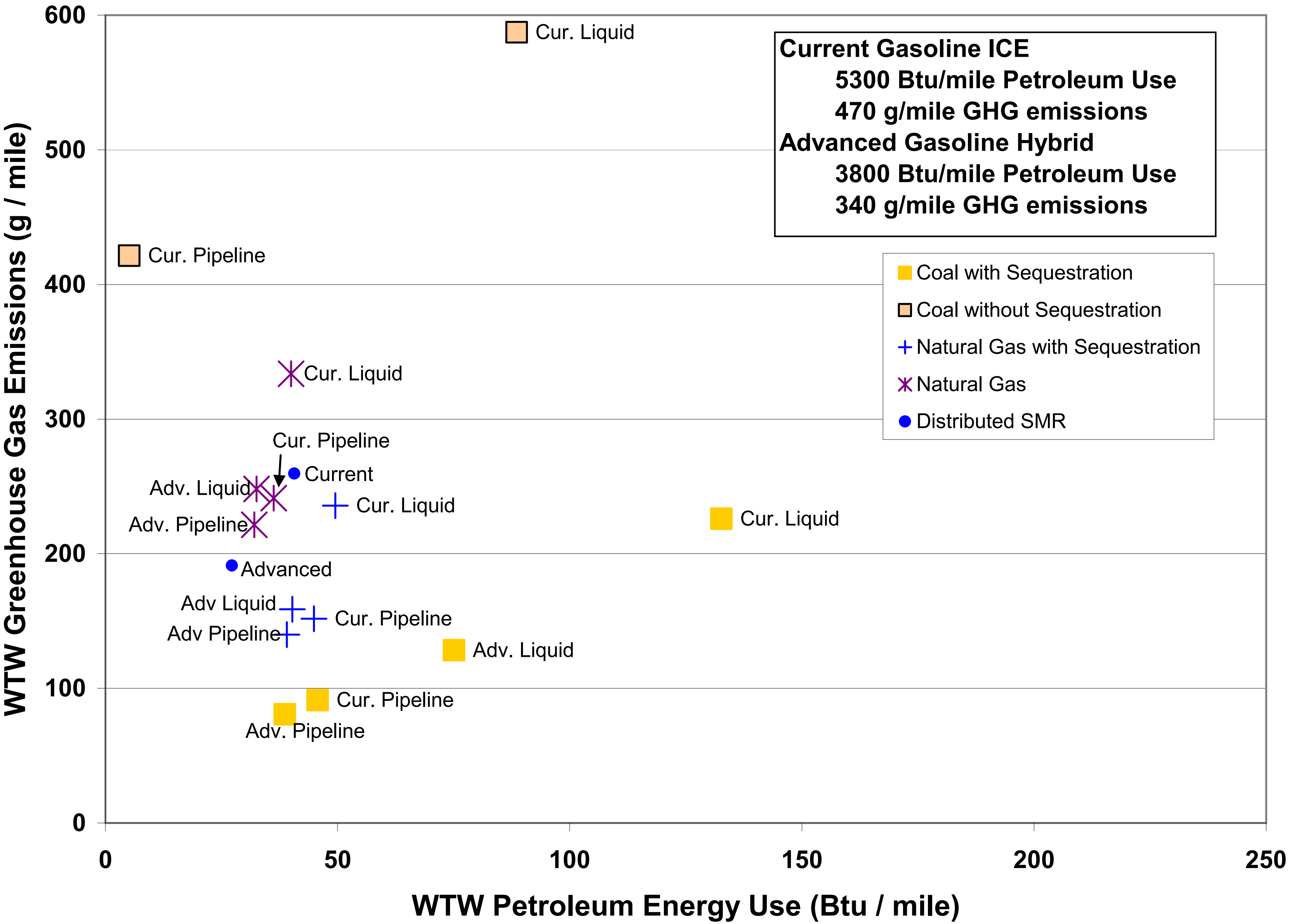

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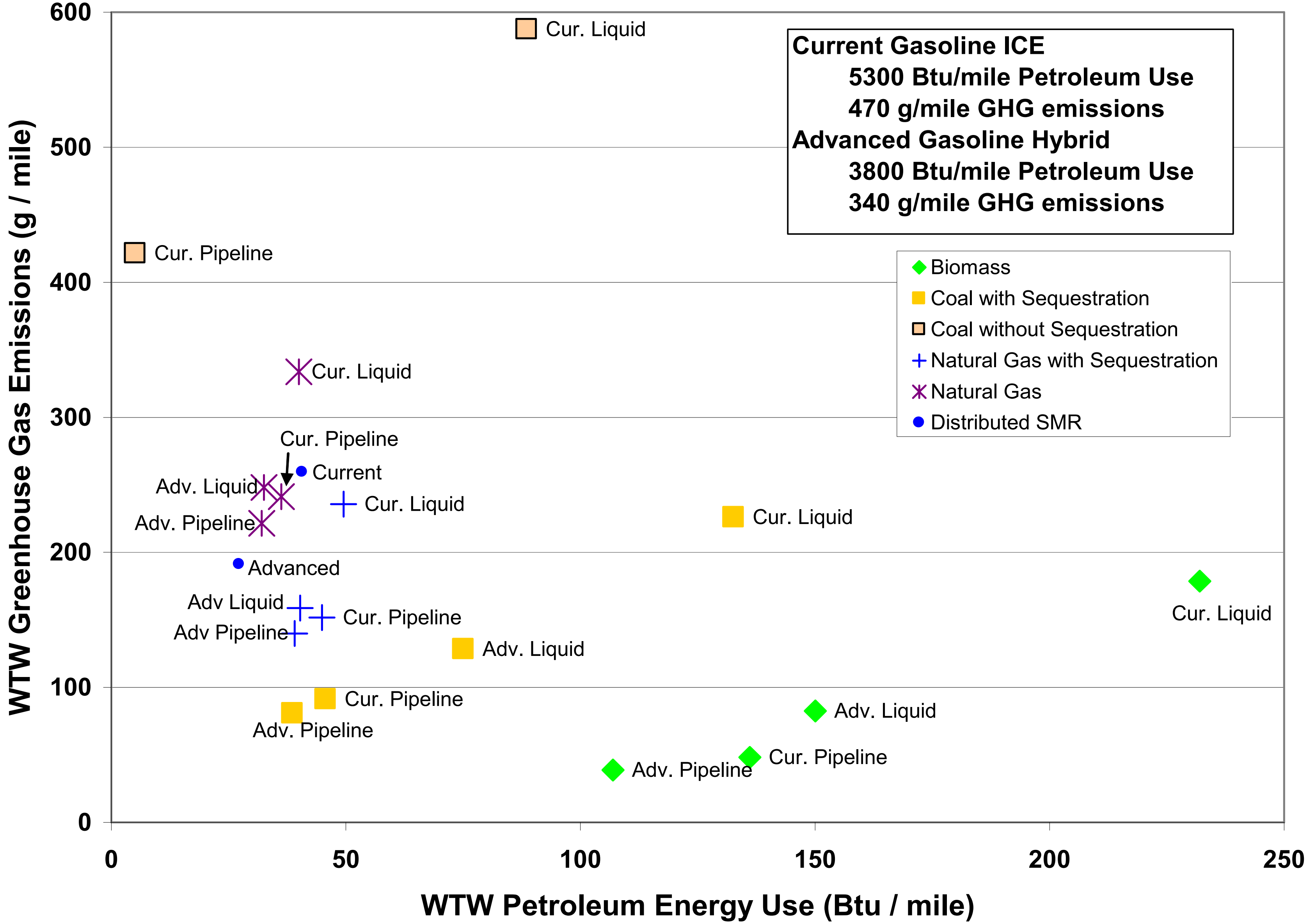

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Progress: Validating Use of Models

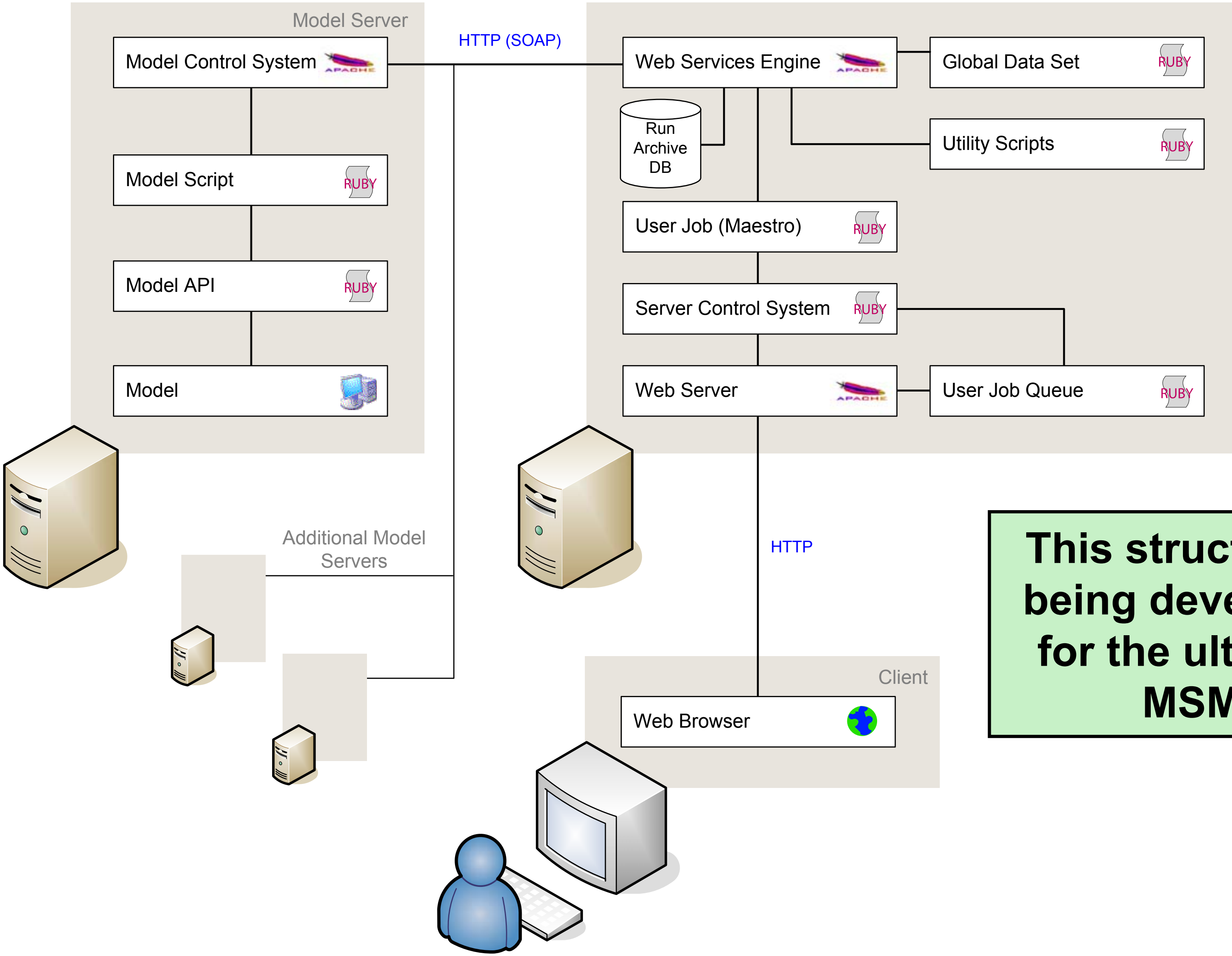
Discussions with Model Developers
- Understand the model's purpose & use
- Compile lists of inputs and results

Understand models intimately
- Definition of terms
- Calculation methodology

Comparison to other analyses
- Meticulous review of inputs & results
- Mapping between results from different analyses
- Distributed SMR, biomass gasification, and coal gasification were mapped to the posture plan
- Other pathways are being compared in the HyWAYS / IPHE project

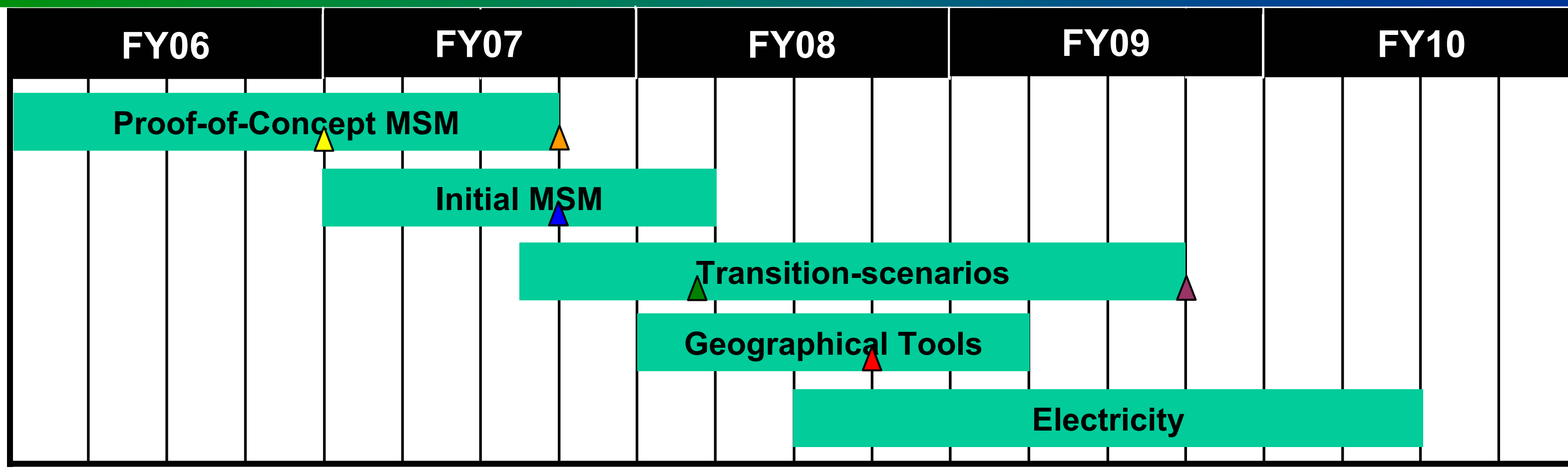
Interaction with community (analysts & industry)
- Present & discuss methods & results
- Reach consensus on approach & parameters

Progress: Extensible MSM Structure



This structure is being developed for the ultimate MSM

Proposed Future Work



- Proof-of-Concept MSM (H2A Production, HDSAM, GREET linked with Excel and Java)
  - Validation of the MSM's interactions with other models
  - Initial analysis of production/delivery pathways (September 30, 2006)
  - Peer-review (June 26, 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 (June 26, 2007)
  - Develop stochastic modeling capability and decision-making tools
- Link transition-scenario models to MSM
  - Determine next set of issues that need to be addressed
  - Link HyPRO to MSM (November 30, 2007)
  - Consider linking HyTRANS or HyDS
  - Review transition scenarios using the MSM (June 30, 2009)
- Link geographical tools to MSM
  - Determine next set of issues that need to be addressed
  - Link HyDRA to the MSM (June 30, 2008)
- Add stationary electrical generation and electrical infrastructure (February 28, 2010)

Summary

- The MSM is being built to address priority analysis issues
- A proof-of-concept version of the MSM exists and is being used for analysis
- H2A Production, HDSAM, and GREET have been linked in the proof-of-concept version of the MSM so pathways can be analyzed
- Use of these models has been validated
- The MSM can perform sensitivity analyses to help the community understand effects of research outputs
- An extensible and user-friendly version of the MSM is being developed

Acknowledgements

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  - Timothy Sa, Keith Vanderveen, Michael Goldsby
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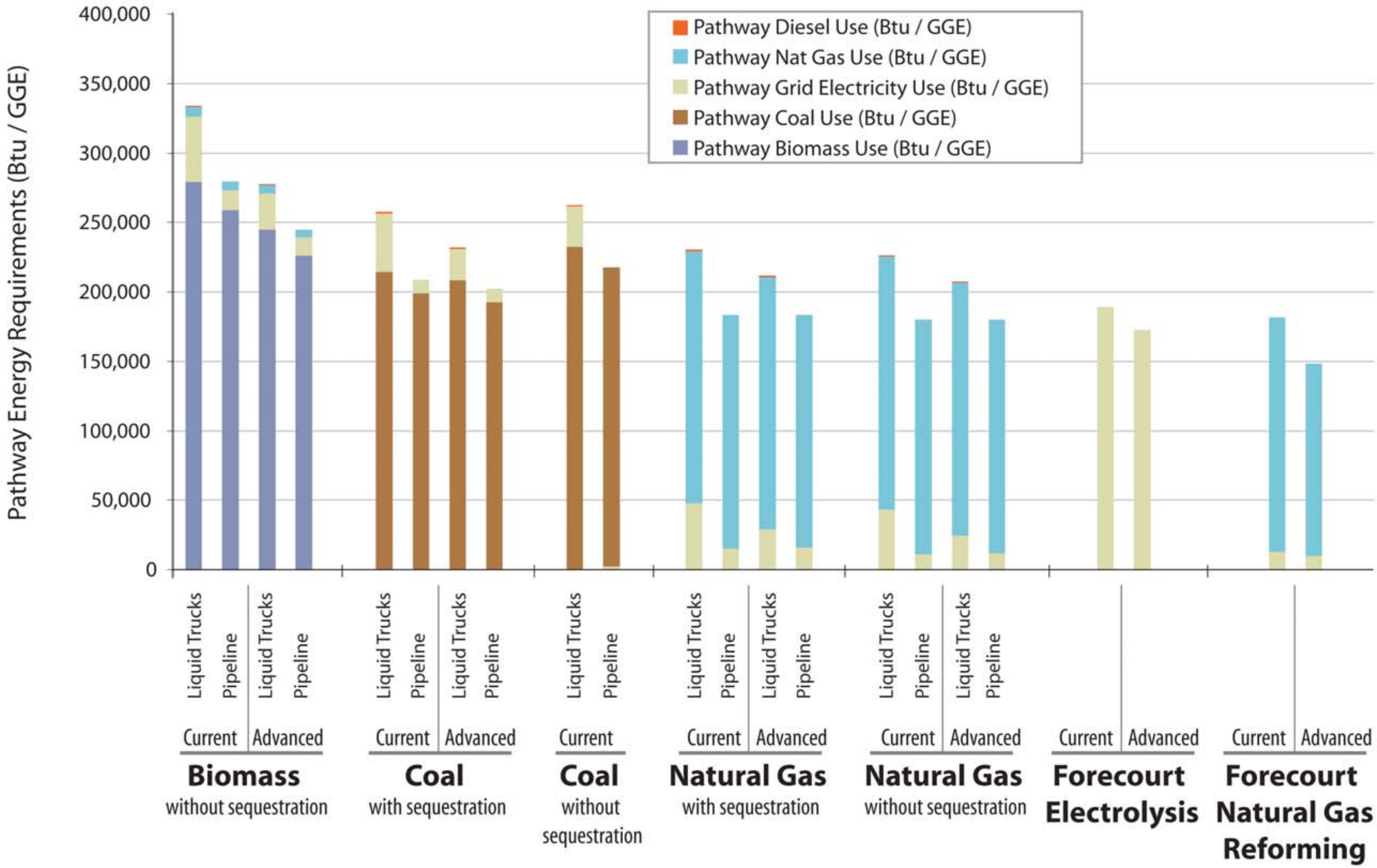
- **Directed Technologies, Inc.**
  - Brian James, Julie Perez

Questions

Pathway Energy Results



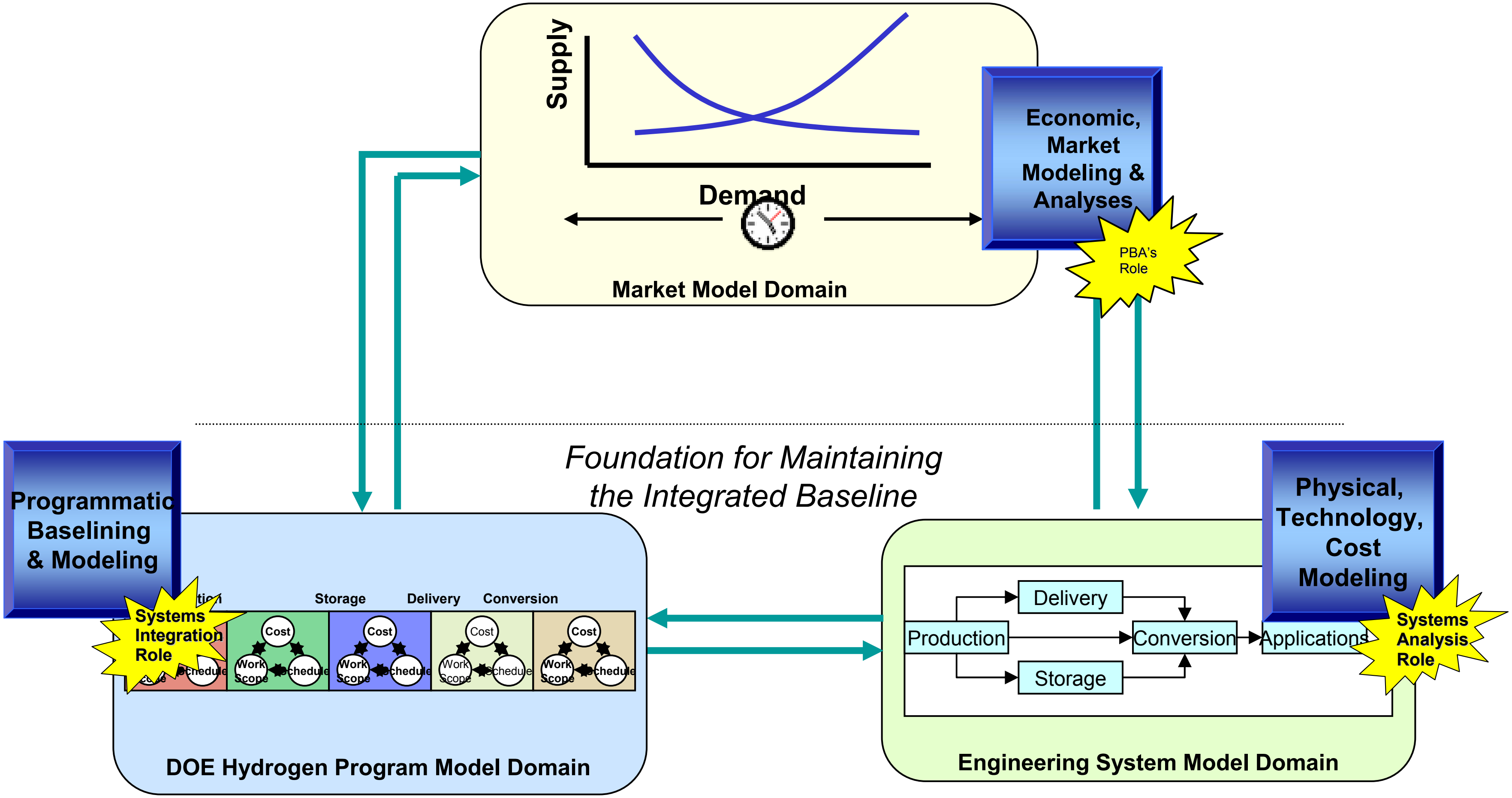
The MSM eases comparisons of pathway energy requirements

Results: Effect of H_2 Losses

Current, Biomass Gasification, Liquid Hydrogen Delivered in Trucks

	H2 losses during delivery	No H2 losses during delivery
Levelized Cost	$5.47 / kg H2 (at pump, pre-tax)	$5.14 / kg H2 (at pump, pre-tax)
WTW Greenhouse Gas Emissions	179 g / mile	166 g / mile
WTW Petroleum Use	232 Btu / mile	215 Btu / mile
WTW Fossil Energy Use	2160 Btu / mile	2000 Btu / mile

Role in EERE Modeling Domain



- **Macro-system model will simulate system performance and enable evaluation of components/interfaces from system level perspective**