Oak Ridge National Laboratory

David L. Greene

Engineering Science and Technology Division

Paul N. Leiby

Environmental Sciences Division

Juan Ferrada

Nuclear Science and Technology Division

DOE Hydrogen, Fuel Cells, and Infrastructure Technologies Program

Systems Analysis Workshop

July 28-29, 2004

Washington, D.C.

Charter

- The Engineering Science and Technology Division, National Transportation Research Center conducts engineering and analytical R&D for DOE, other federal sponsors and the private sector.
- The Environmental Sciences Division conducts interdisciplinary research, develops technology, and performs analyses to understand and assess responses to global and regional change, environmental stress, and resource use.
- TPP carries out research, modeling and analysis for DOE and other federal sponsors.
  - DOE – Modeling and analysis of fuel economy standards, Transition Alternative Fuels and Vehicles Model, Refinery Impacts Modeling for reformulated fuels, costs of oil dependence, SPR optimization.
  - EIA – Model development for NEMS Transportation Sector
  - DOD – Airlift Deployment Analysis System, Defense Logistics
  - DOT – Modeling, Forecasting and Analysis of Freight Flows, Vehicle Travel Forecasting, Traffic Simulation and Optimization

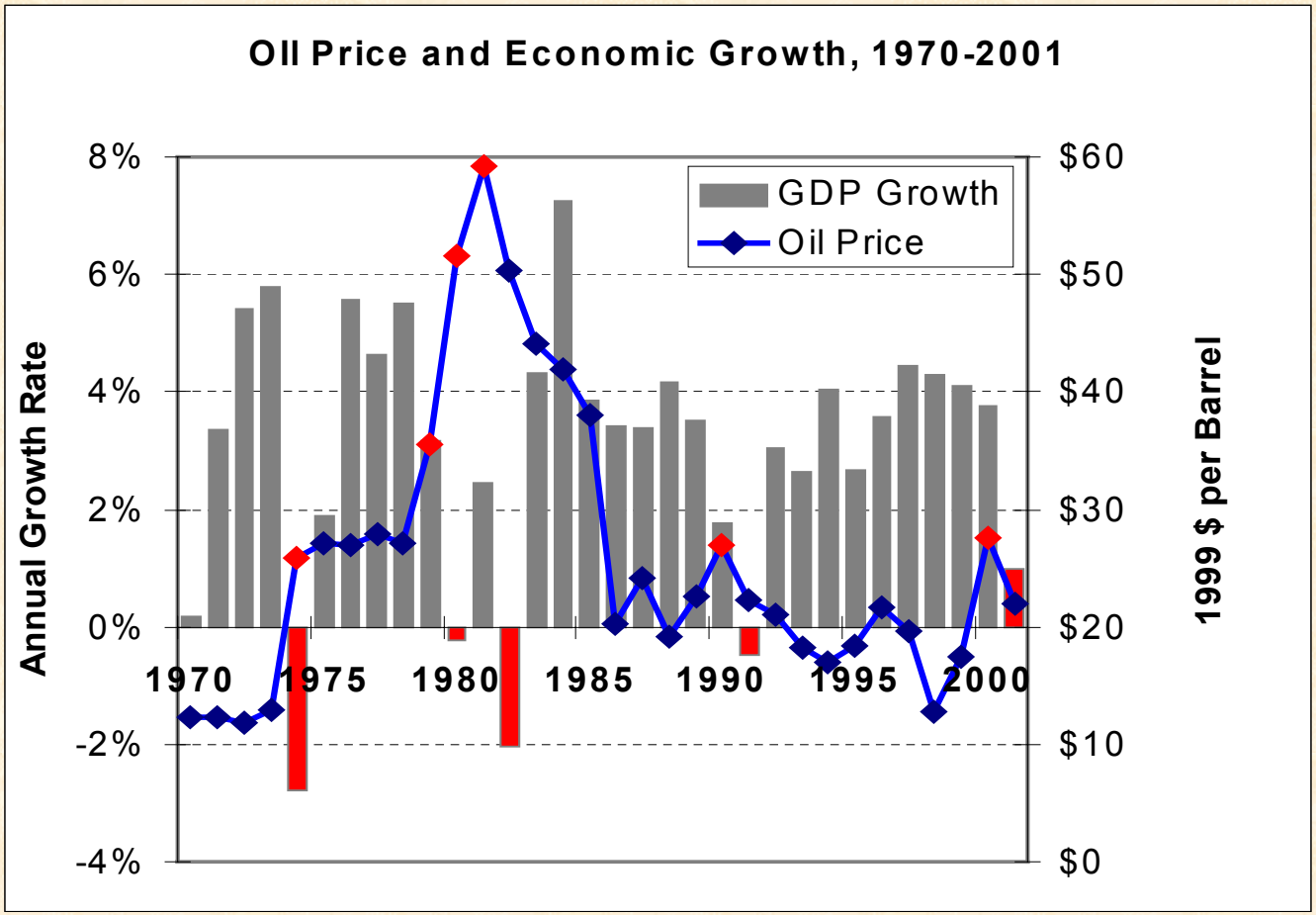
History

- ***ORNL's Transportation Energy Group began modeling and analysis R&D in 1980.***
- ***Transition Alternative Fuels and Vehicles Model: Analysis of EPACT alternative fuels targets, expanded private fleet rulemaking.***
- ***World Energy Scenarios Model: DOE/NRCanada 2050 Study.***
- ***NEMS Alternative Fuel Vehicle Choice Model: currently incorportated in NEMS.***
- ***We are relatively new to hydrogen, having begun our transition in 2002.***

Transportation policy and planning continues a 25-year research program at ORNL.

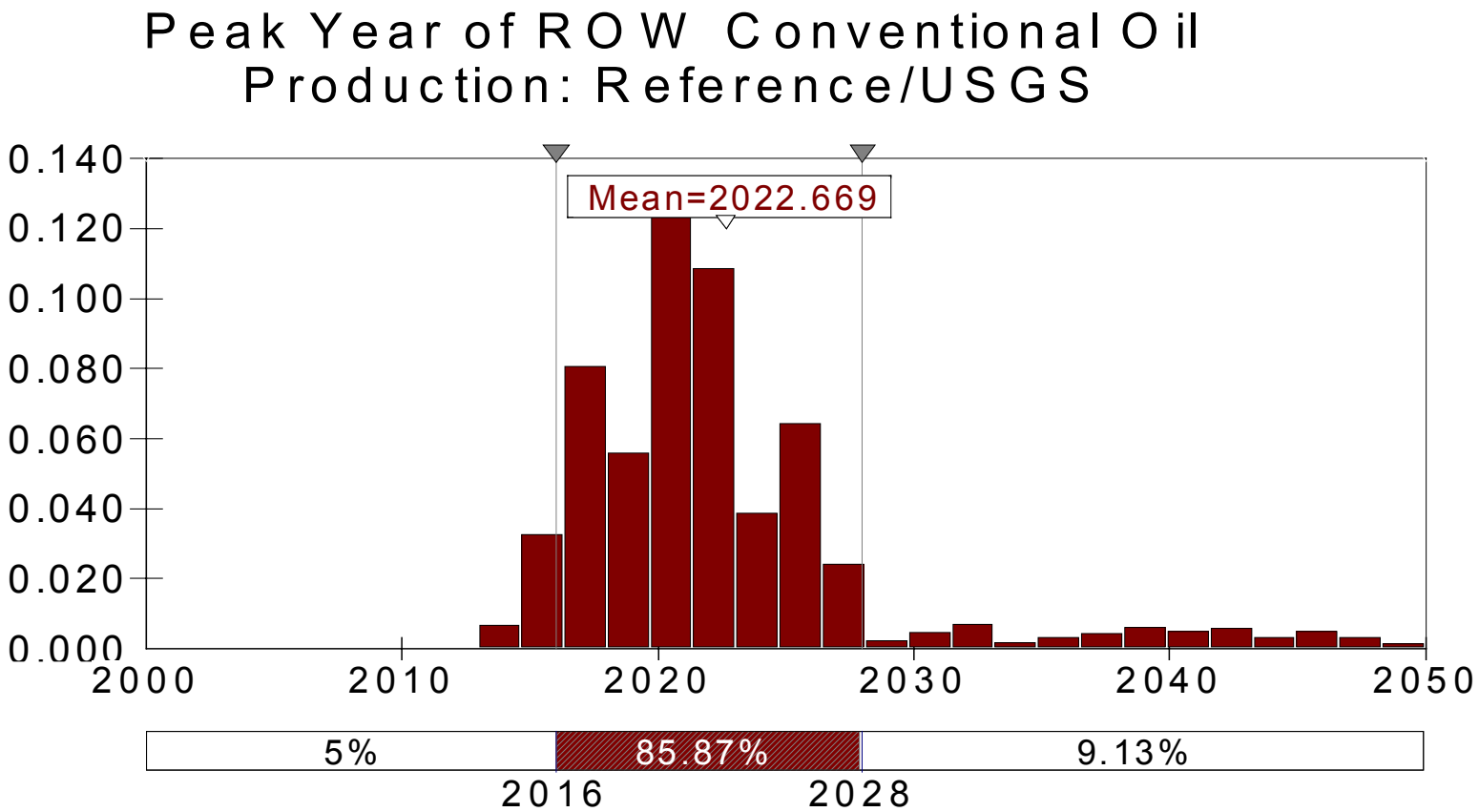
- Energy Policy Analysis
  - Fuel Economy Policy Analysis
  - Oil Dependence Analysis
  - Greenhouse Gas Mitigation
  - Fuel Economy Information Program (Clean Cities)
  - Hydrogen Transition (HYTRANS) Model
  - Hydrogen Education and Outreach
- Planning and Operations
  - Solving Defense Logistics and Problems Since 1982
  - Travel and Traffic Modeling
  - Freight data and freight activity modeling
  - Transportation security analysis
  - Safety studies

We have developed and implemented methods for estimating the economic costs of oil dependence.

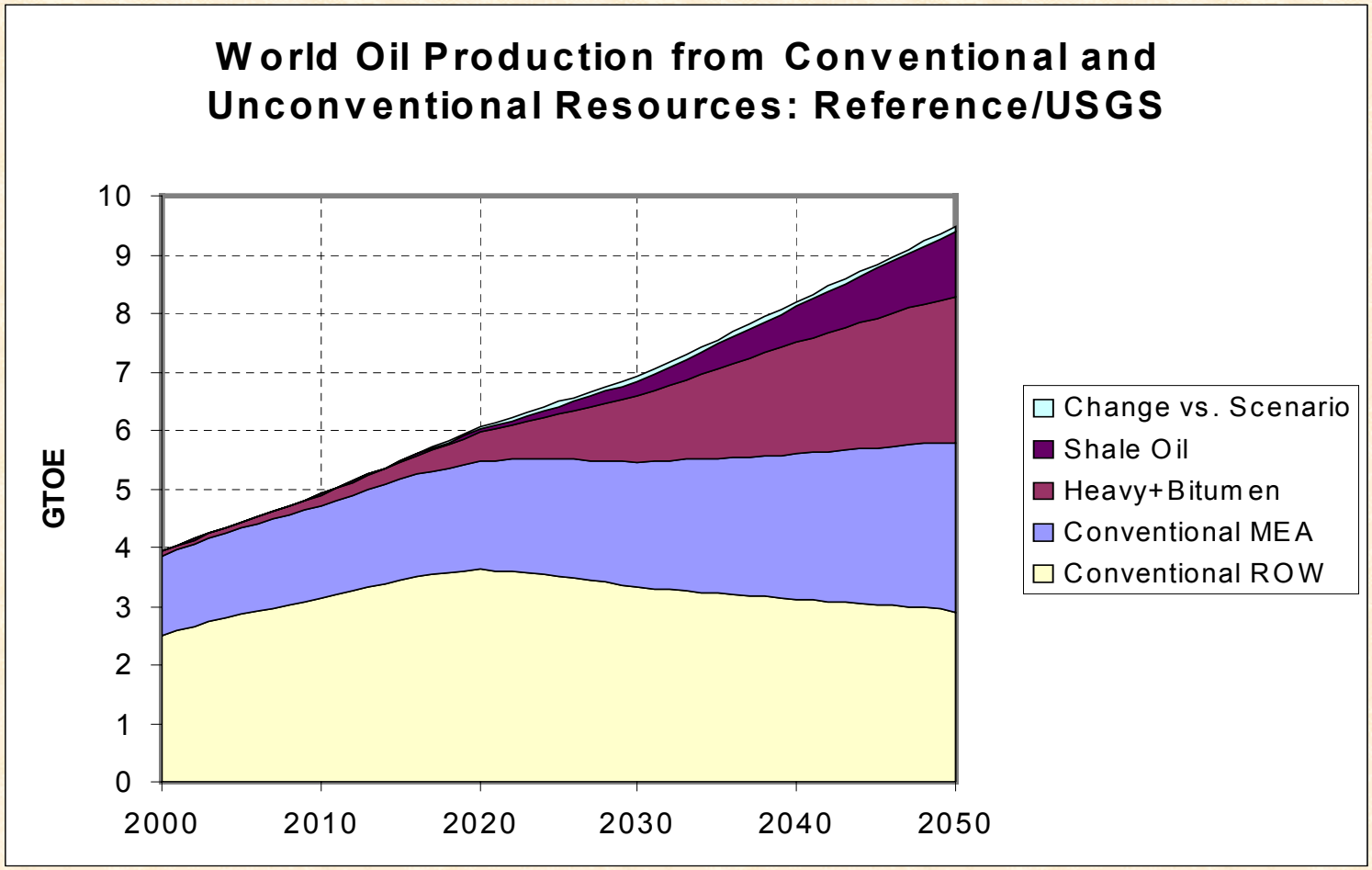


"…at least the last three recession periods in the United States – those of 1990-91, 1980-82 and 1974-75 – were preceded by spikes in the price of oil." Alan Greenspan, June 28, 2001

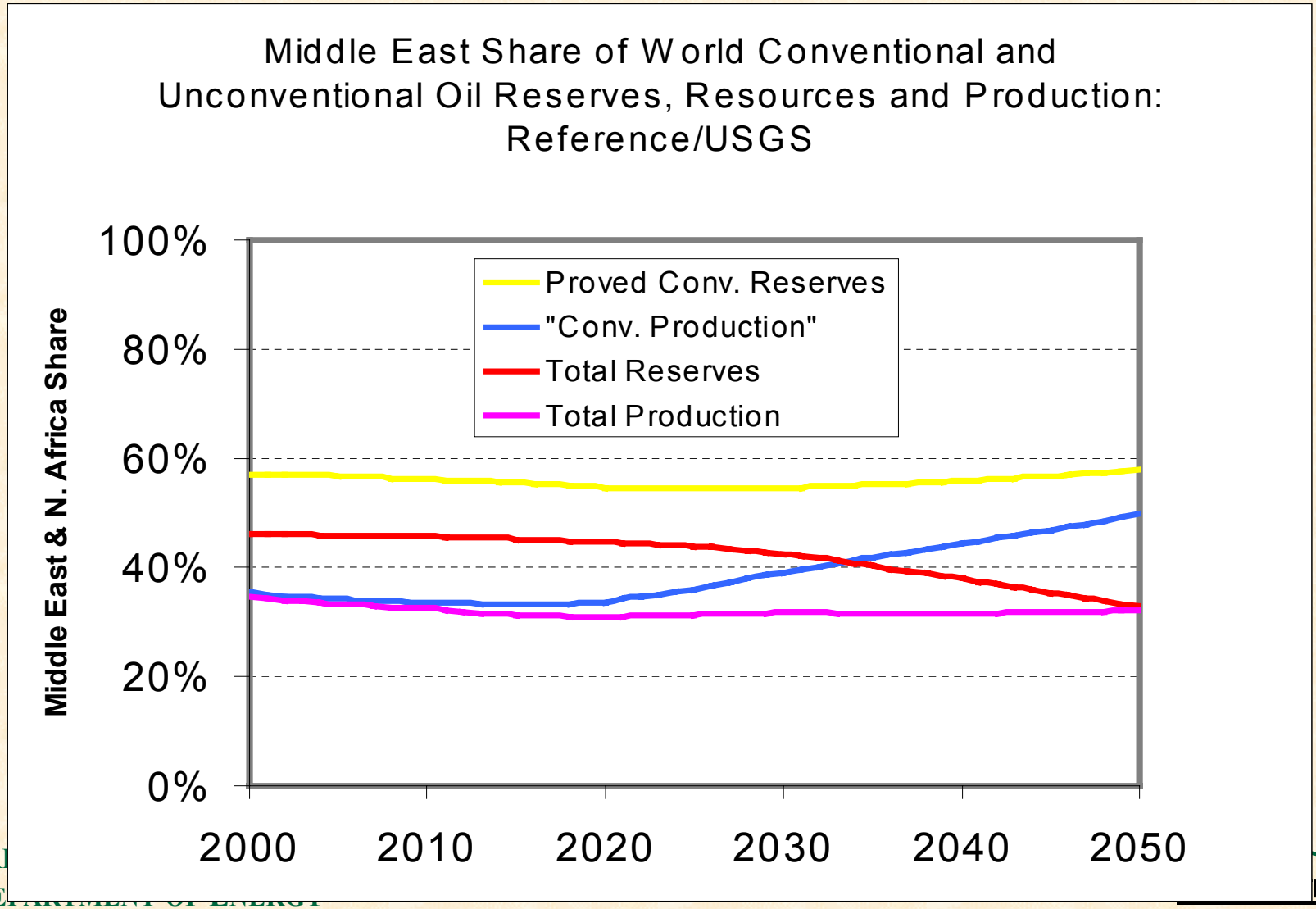
Using world energy scenarios and methods of risk analysis, we have analyzed the timing of the peaking of conventional oil supplies and a transition to unconventional supplies.



Under median assumptions, unconventional oil production must expand rapidly after 2020.



Even with a global transition to unconventional oil resources, the Middle East could maintain a dominant position through 2050.



ORNL has been developing transportation and logistics systems for DOD since 1982.

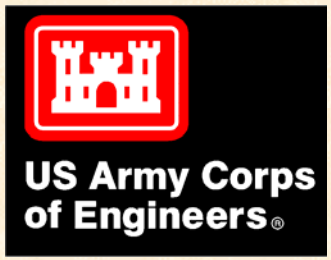
MOBCON

SAIL
SEASTRAT

ADANS

SCM
MICLOG

IBS
WPS
STRADS
TOPS
TCACCIS
WHISTMOD



ORNIM

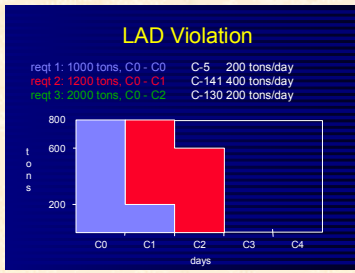
ALRM
OSCAR

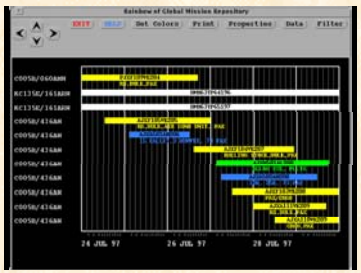
JFAST

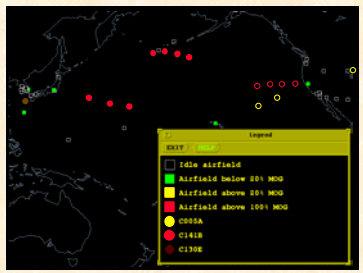
ALP

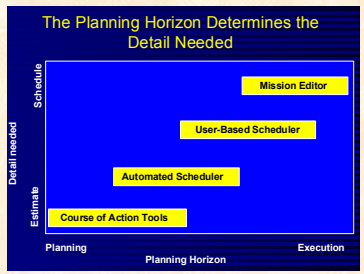
Developer of the AMC Deployment Analysis System (ADANS)

- Operational in early 1990 planning and scheduling worldwide airlift for DoD
- Scheduled the largest airlift in history (DESERT STORM)
- Scheduling algorithms, centralized database, and a suite of flexible analysis tools

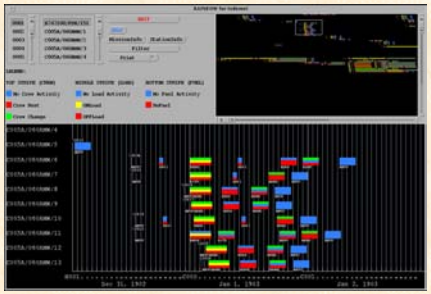


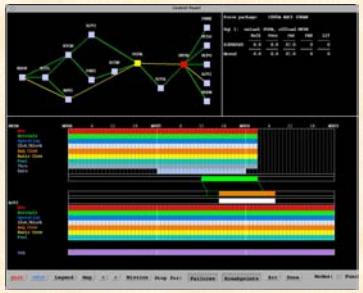


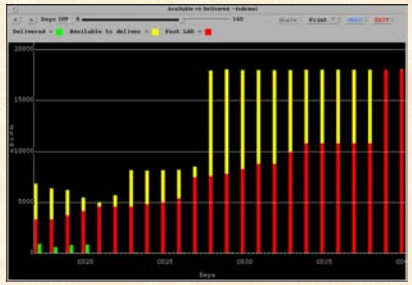




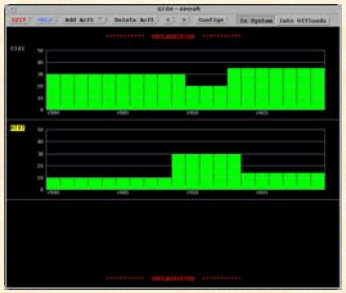
Consolidated Air Mobility Planning and Scheduling (CAMPS)

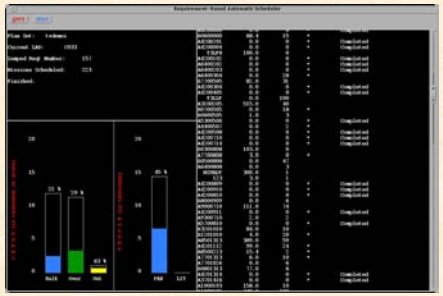


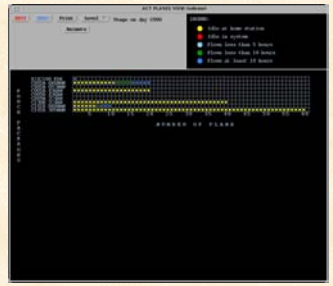




CAMPS scheduling tools are AMC's means of scheduling major military operations like *Enduring Freedom* and *Iraqi Freedom*







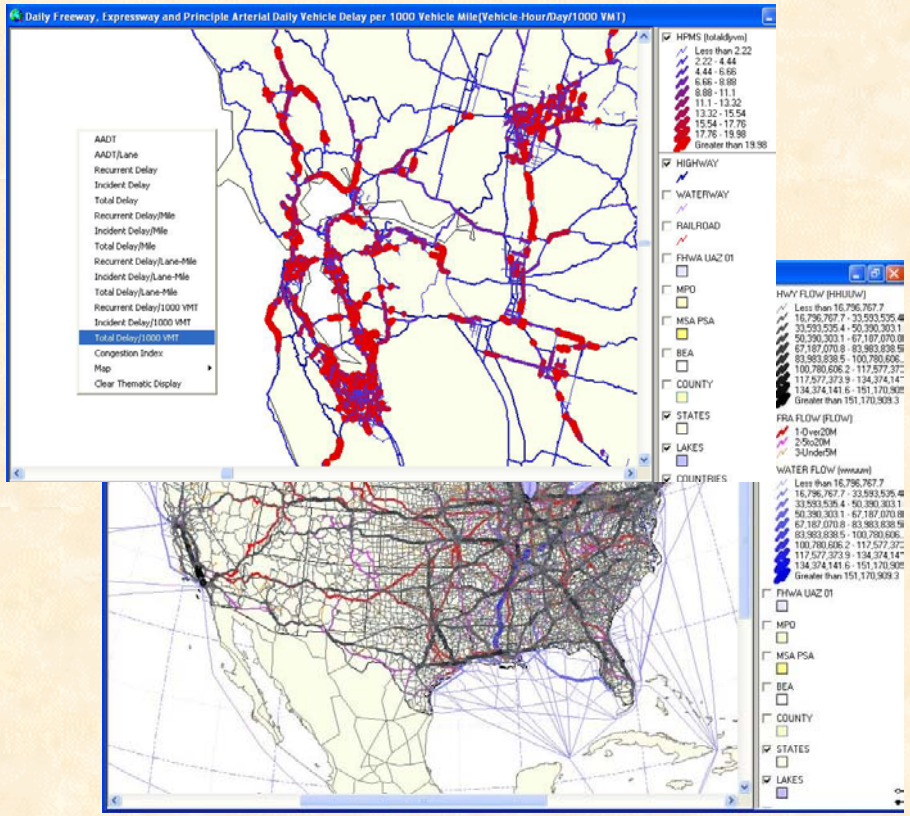
Ohio River Navigation Investment Model

- **A spatially-detailed partial equilibrium model**
- **Built by ORNL in collaboration with the U.S. Army Corps of Engineers' Center of Excellence in Navigation Planning**
- **Estimates** net economic benefits **of river system infrastructure improvements**
  - **New locks/Lock extensions**
  - **Maintenance plans**
  - **Operations policies**

GeoFreight

Is A Multi-Modal, GIS-Based Freight Analysis & Display Software Used To:

- **Estimate flows of domestic & international freight across the nation**
- **Assess current and potential major freight bottlenecks in the transportation system**



TAFV Project Identified and Modeled Key Transitional "Barriers"

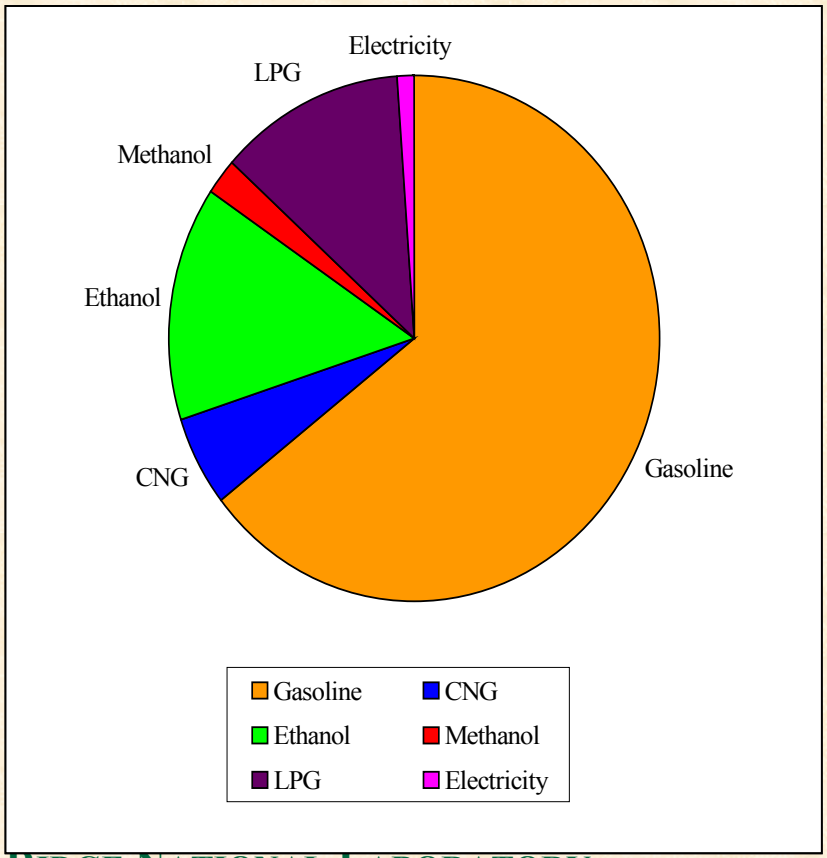
- Vehicle and fuel infrastructure requirements large, and not explicitly coordinated
- Fuel Availability
  - Alternative fuels rarely available (at filling stations)
- Scale economies:
  - Initial vehicle costs high (at low production scales)
- Limited vehicle model diversity
  - New tech available on only a few vehicle makes
- Possible Learning from production experience
- Slow capital stock turnover

TAFV

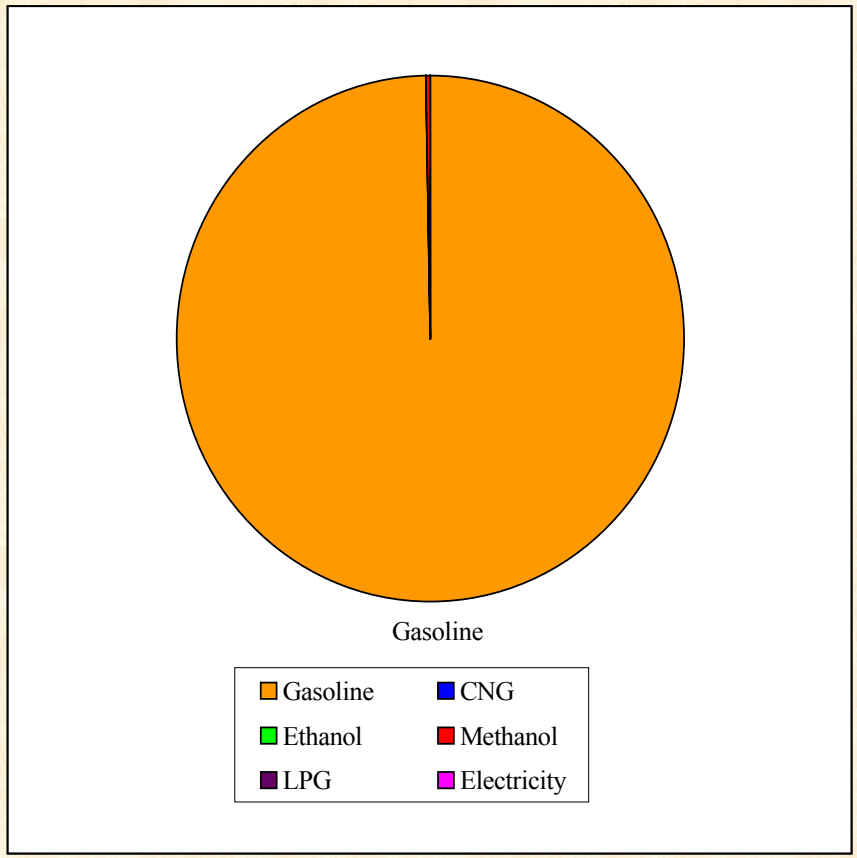
Find: Barriers to Alt Fuels Real & Important

2010 Alternative Fuel Demand Shares, Base Case (No New Policy)

No Transitional Barriers



Transitional Analysis With Barriers



(Base Case, No New Policies AEO HWOP, Lower LPG Cost)

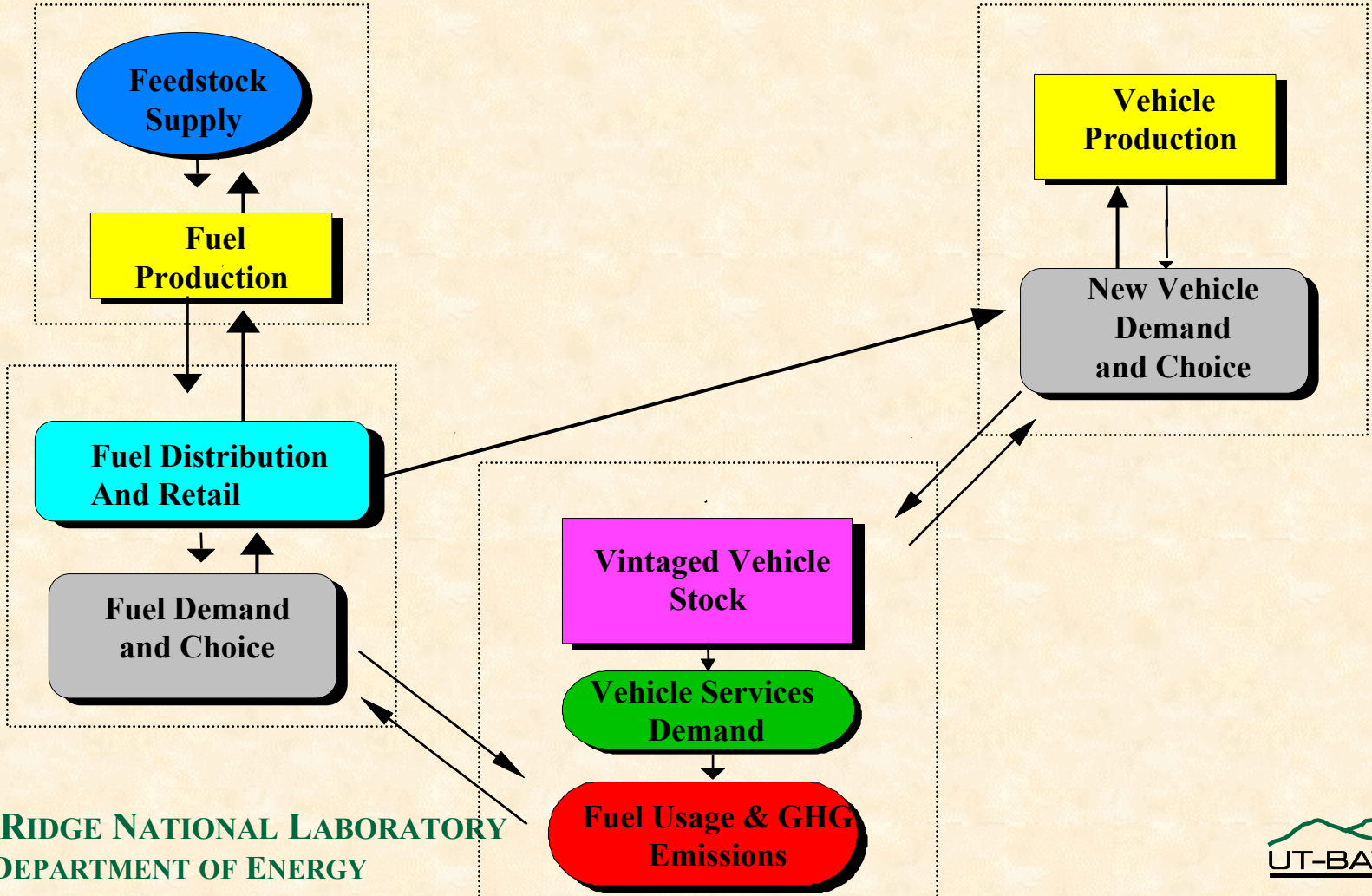
Working together with teams from other National Laboratories, academia and industry, ORNL is helping to create analytical tools for understanding the transition to a hydrogen economy.

- In what scenarios (under what conditions) will the hydrogen economy succeed?
- How do individual technologies affect the transition to and functioning of the system?
- How do alternative energy sources affect the transition to and functioning of the system?
- How will the evolution of the system over time and geographically affect costs and benefits?
- What is the role for policy in the transition and maintenance of the hydrogen economy?
- What are the costs and benefits (including the global macroeconomic effects) of a hydrogen economy?

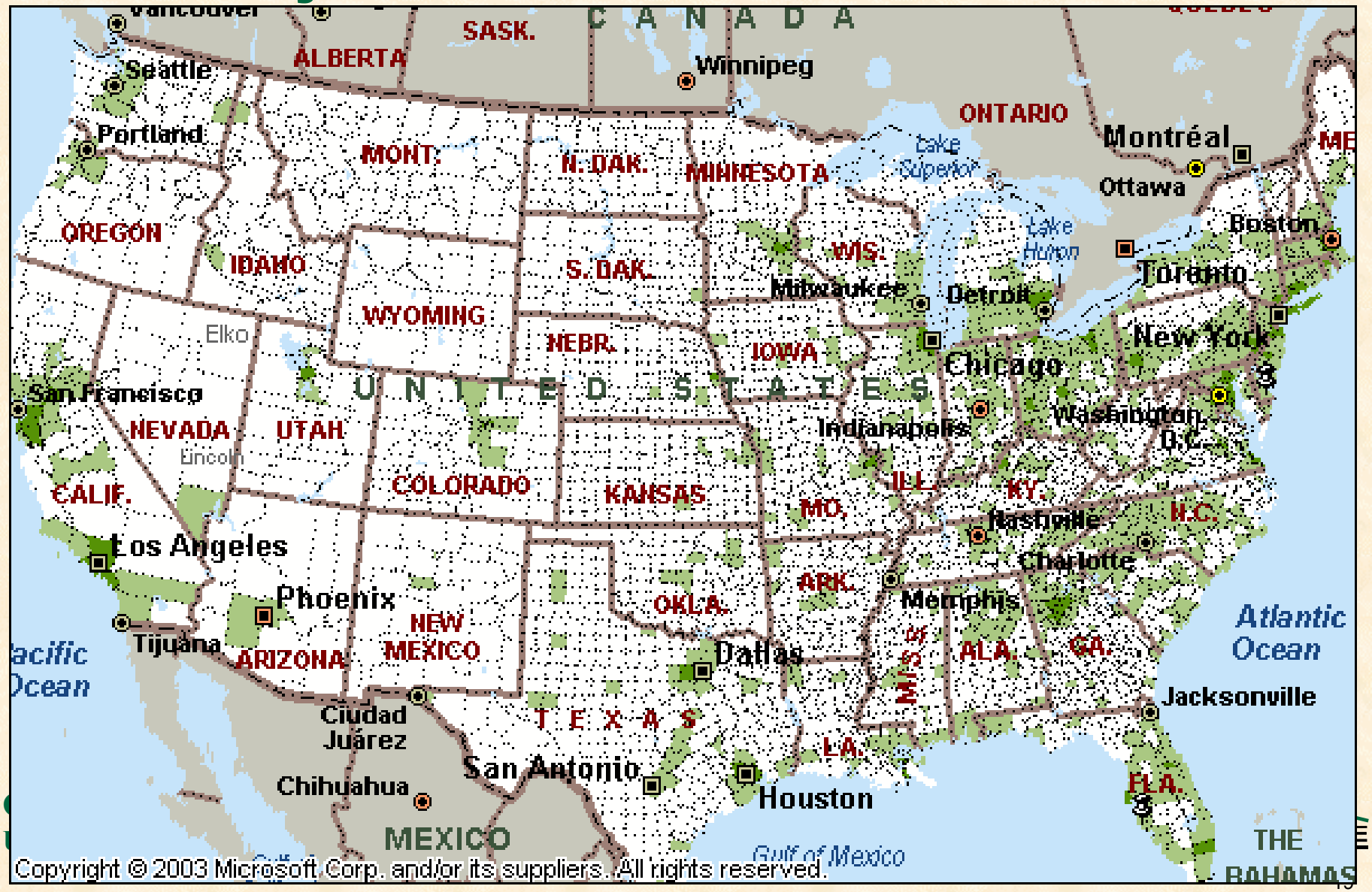
Approach: HyTrans applies optimization methods to construct an economic model of the hydrogen transition.

- Represents interdependent decisions of hydrogen suppliers, vehicle manufacturers & consumers from 2000 to 2050.
- Finds competitive market solutions by maximizing producers' profits and consumers' welfare.
- Decision-making to 2050 can be based on perfect foresight, myopia, or other expectation models.
- Version 1 is limited in scope.
  - Only 3 production technologies
    - Centralized SMR
    - Forecourt SMR
    - Forecourt Electrolysis
  - Considers only LDV H2 demand
  - National, aspatial market structure

HyTrans finds a simultaneous solution that integrates consumer, fuel producer, fuel distributor and vehicle manufacturer decisions.



A key factor in infrastructure evolution will be the density of motor fuel demand. In HyTrans there are three markets.



What's next?

- National version operational on SFA data.
- Added NAS data June, 2004.
- Improving representation of fuel availability and driver response (Melaina).
- Adding H2A data ASAP.
- Running and documenting national transition scenarios, Sept 2004.
- Adding Census regions, Dec. 2004.

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Nuclear Science and Technology Division

Juan J. Ferrada, PhD

Principal Investigator

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- ***Organization's Mission***

  The Nuclear Science and Technology Division performs basic and applied R&D for the Department of Energy, the National Nuclear Security Administration, and other government agencies, as well as supporting and leveraging industrial partnerships.

- ***Group's mission***

  The Process Engineering Research Group performs R&D and systems analysis in support of verification, design, development, and operation of energy related processes and equipment.

Charter (continued)

Past funding

- ***DOE Mixed Waste Focus Area: $400K***
- ***DOE Mixed Waste Integrated Program: $350K***
- ***DOE Transportable Vitrification System: $100K***
- ***CRADA with SEPRADYNE: $300K***
- ***Non-Proliferation: $250K***
- ***Pu Vitrification System: $80K***
- ***Space Power Options: $100K***
- ***Liquid Low Level Waste Treatment Options: $100K***

Charter (continued)

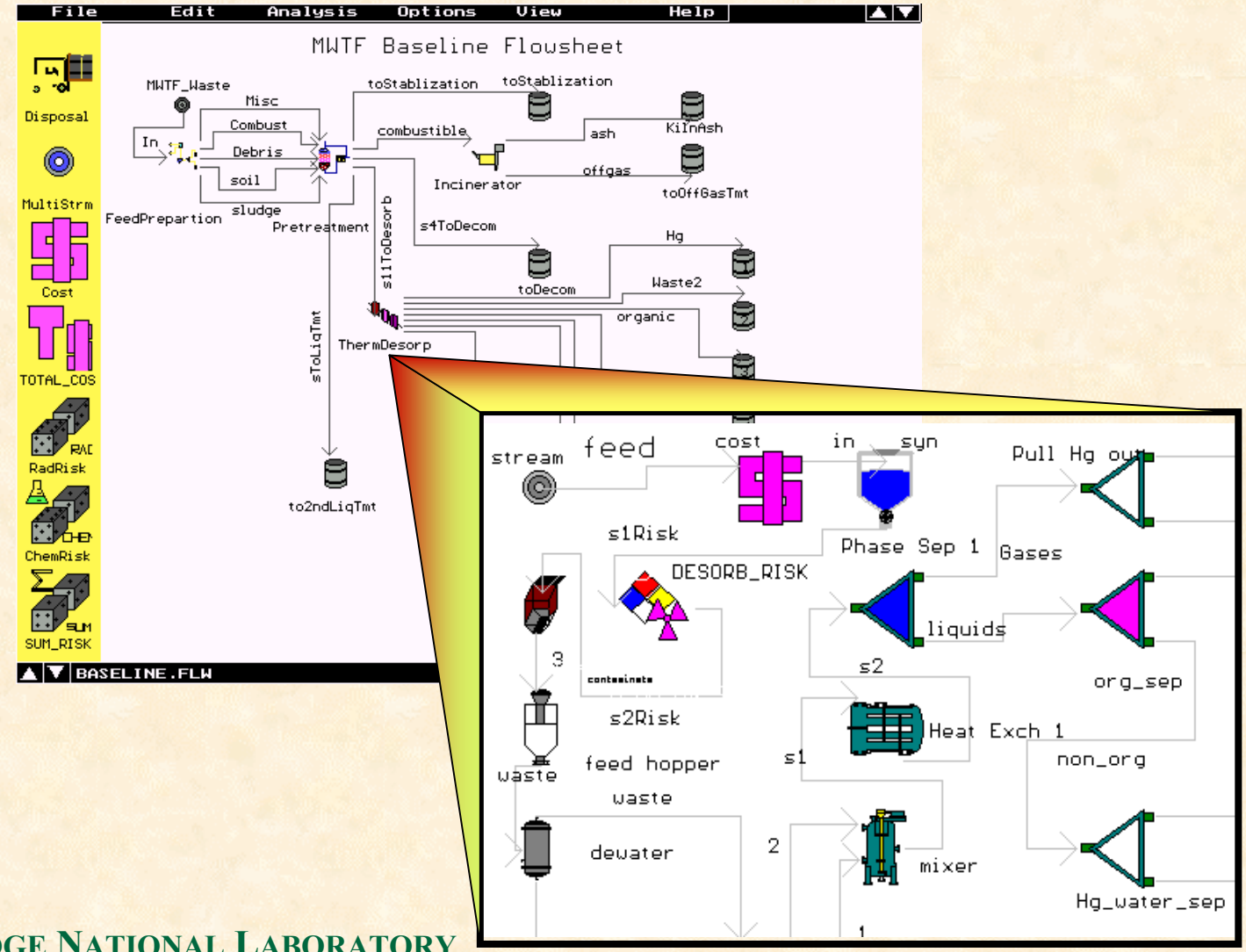
Exploratory Funding

- ***Hydrogen Economy System Demo: $30K***
- ***Hydrogen Production Using TVA Off-peak power: $20K***
- ***Hydrogen Production Using a Novel Thermochemical Cycle: $50K***
- ***Hydrogen Storage and Recycle System using NaBH4: $80K***

History

- ***Our group is doing analysis for the past 15 years***
- ***Significant past analysis projects include the following:***
  - ***Mixed Waste Focus Area: DOE Wixed Waste Systems Analysis***
  - ***Mixed Waste Integrated Program: Multicriteria Evaluation Methodology***
  - ***Engineering Assessment for the DOE Transportable Vitrification System***
  - ***Hg Recuperation from the Copper Industry: CRADA***
  - ***Uranium Conversion Process: Non-Proliferation***
  - ***Innovative Technology Performance Assessment: Pu Vitrification System***
  - ***Liquid Low Level Waste Treatment Alternative***
  - ***Fuel Cycle Flowsheet Analysis for both Domestic and International Sponsors***
  - ***Alternatives for Tank Waste Disposal at ORNL***
  - ***Life Cycle Analysis Projects***
  - ***H_2 Economy Integration/Systems Analysis: Demo Seed Money***
  - ***H_2 Production from TVA's Off-Peak Electric Production***
  - ***H_2 Production from Thermo Cycle process***
- ***We have considered H_2 for the last 3 years***

FLOW, Basic Computerized Platform for Systems Analysis



Skill Set - People

Analysts that helped develop our group's capabilities

- ***Irvin Osborne-Lee, Chem. Eng. PhD,Texas A&M University***
- ***Tim Welch, Chem. Eng. ORNL***
- ***Jim Nehls, MBA, Y-12***
- ***Hom-Ti Lee, Chem, Eng. PhD, K25***
- ***Jason Giardina, Chem. Eng. University of Kentucky***
- ***Ethan Turner, Chem. Eng. University of Tennessee***
- ***Juan J. Ferrada, Chem. Eng, PhD, ORNL***
- ***Les R. Dole, Physical Chem. PhD, ORNL***

Skill Set - People

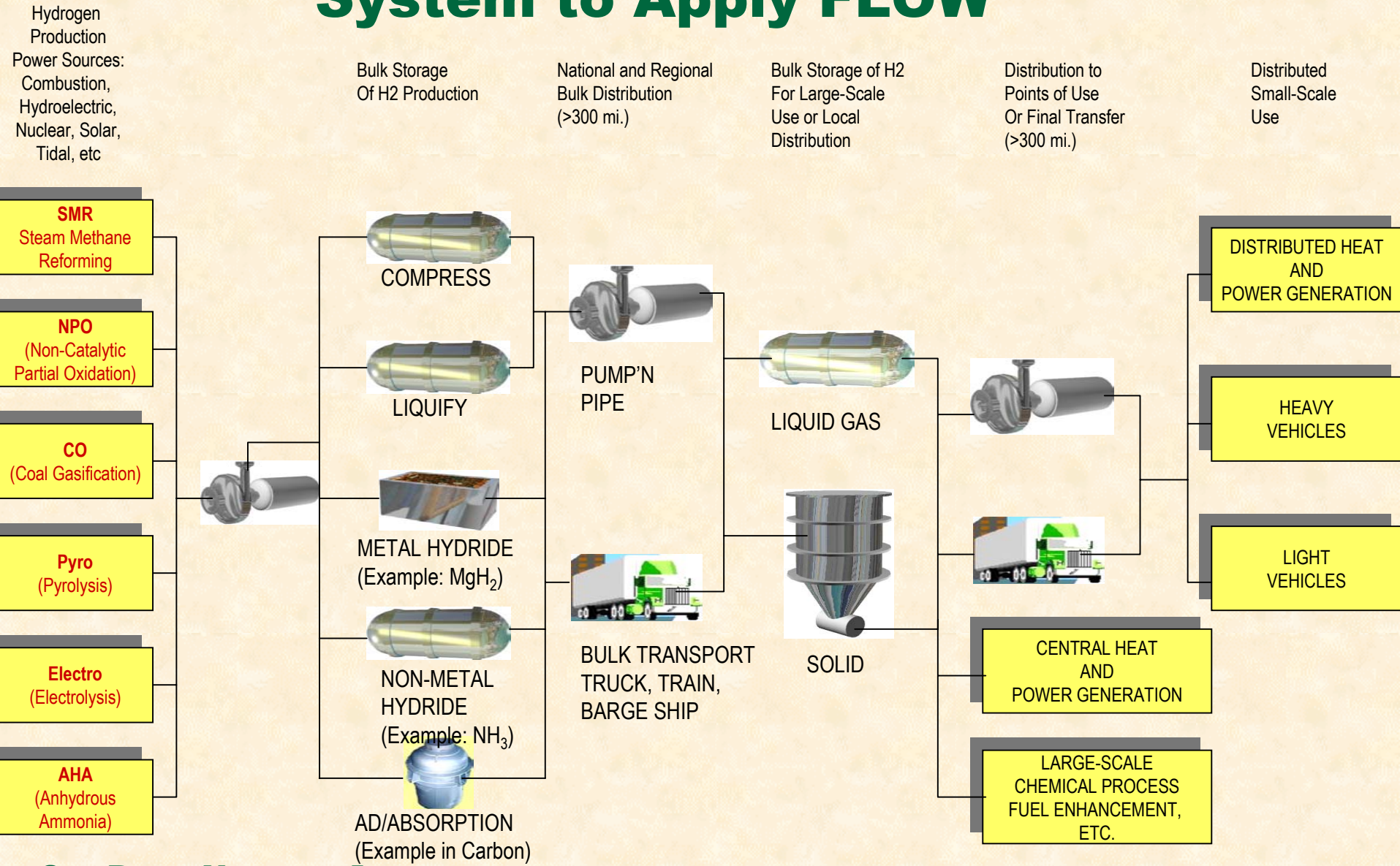
Current analysts

- *Juan J. Ferrada, Chem. Eng. PhD, ORNL, process modeling, cost analysis, evaluation, management, integration*
- *Les R. Dole, Physical Chemistry, PhD, ORNL, thermodynamics, process development, evaluation, integration*
- *David Keffer, Chem. Eng. PhD, University of Tennessee, Molecular Modeling*
- *Darlene K. Slattery, PhD, University of Central Florida, Fuel Cells, Storage, Solar Energy*
- *Tim Armstrong, Materials Science, PhD, ORNL, Fuel Cells, Separation, Management*
- *Beth Armstrong, Materials Science, Master Sc., ORNL, Advanced Process and Manufacturing*
- *Joe Birdwell, Chem. Eng. PhD, ORNL, process verification, process development, process evaluation*
- *Joe Walker, Chem. Eng. ORNL, management, process development*
- *Ben Lewis, Chem. Eng. ORNL, management, process verification*

Skill Set – Models that include H_2

- ***H_2 System including Reforming and Shifting, Piping, and Storage***
  - ***2003***
  - ***System integrates H_2 production, PSA purification, compressing and piping, and Storage. Estimates production, production costs, can optimize piping system.***
  - ***Models are based on thermodynamic, heuristics, and mass and energy balance. Cost models are programmed into system (ENREL, LBNL, LLNL, German, Sandia models).***
  - ***Model platform FLOW accessing HSC5 equilibrium models.***
  - ***Limitations: Does not have large thermodynamic databases, but may import from other programs.***

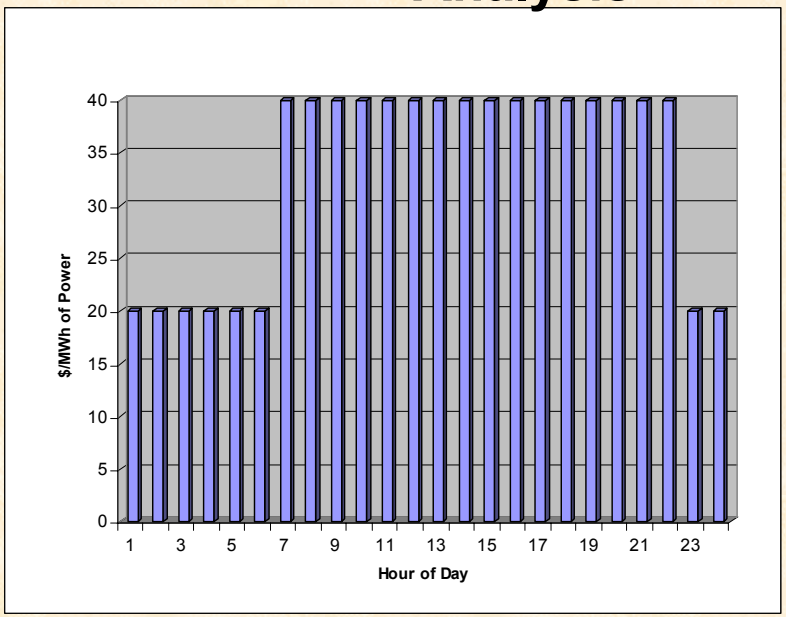
System to Apply FLOW

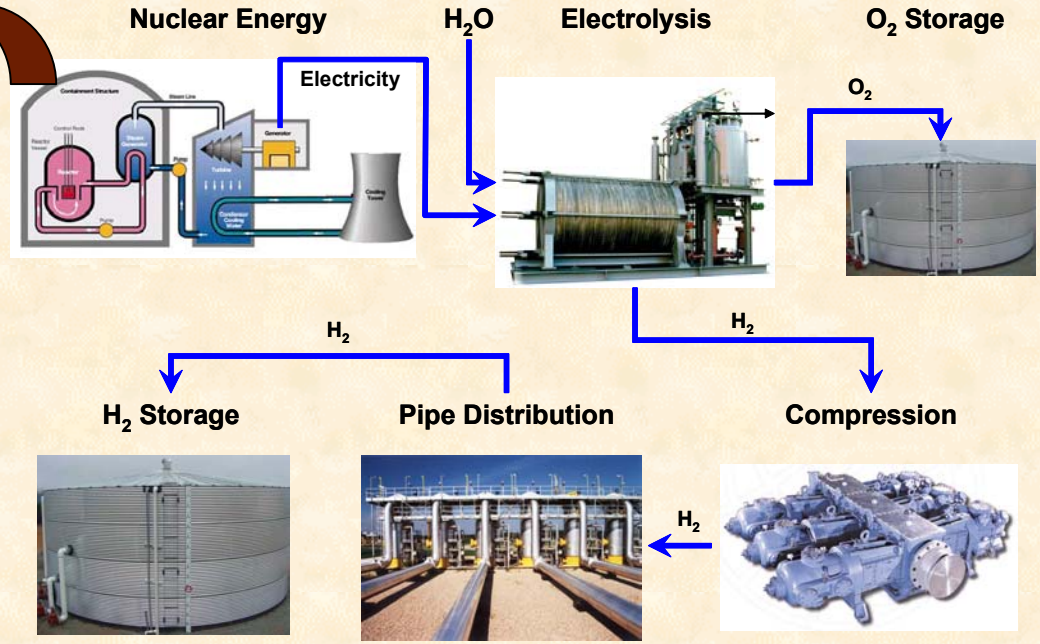


Skill Set – Models that include H_2 (continued)

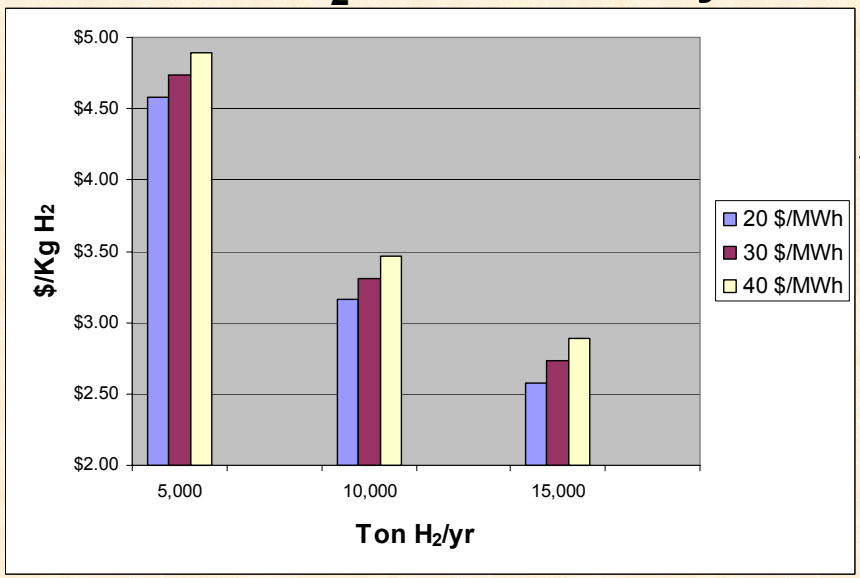
- ***H_2 System including Electrolysis Using TVA Off-peak Power, Piping, and Storage***
  - ***2004***
  - ***System integrates H_2 production by electrolysis, compressing and piping, and Storage. Estimates production, production costs, can optimize piping system.***
  - ***Models are based on thermodynamic, heuristics, and mass and energy balance. Cost models are programmed into system (ENREL, LBNL, LLNL, German, Sandia models, vendors).***
  - ***Model platform FLOW accessing HSC5 equilibrium models.***
  - ***Limitations: Does not have large thermodynamic databases, but may import from other programs***

Off-peak Analysis





H_2 Production System



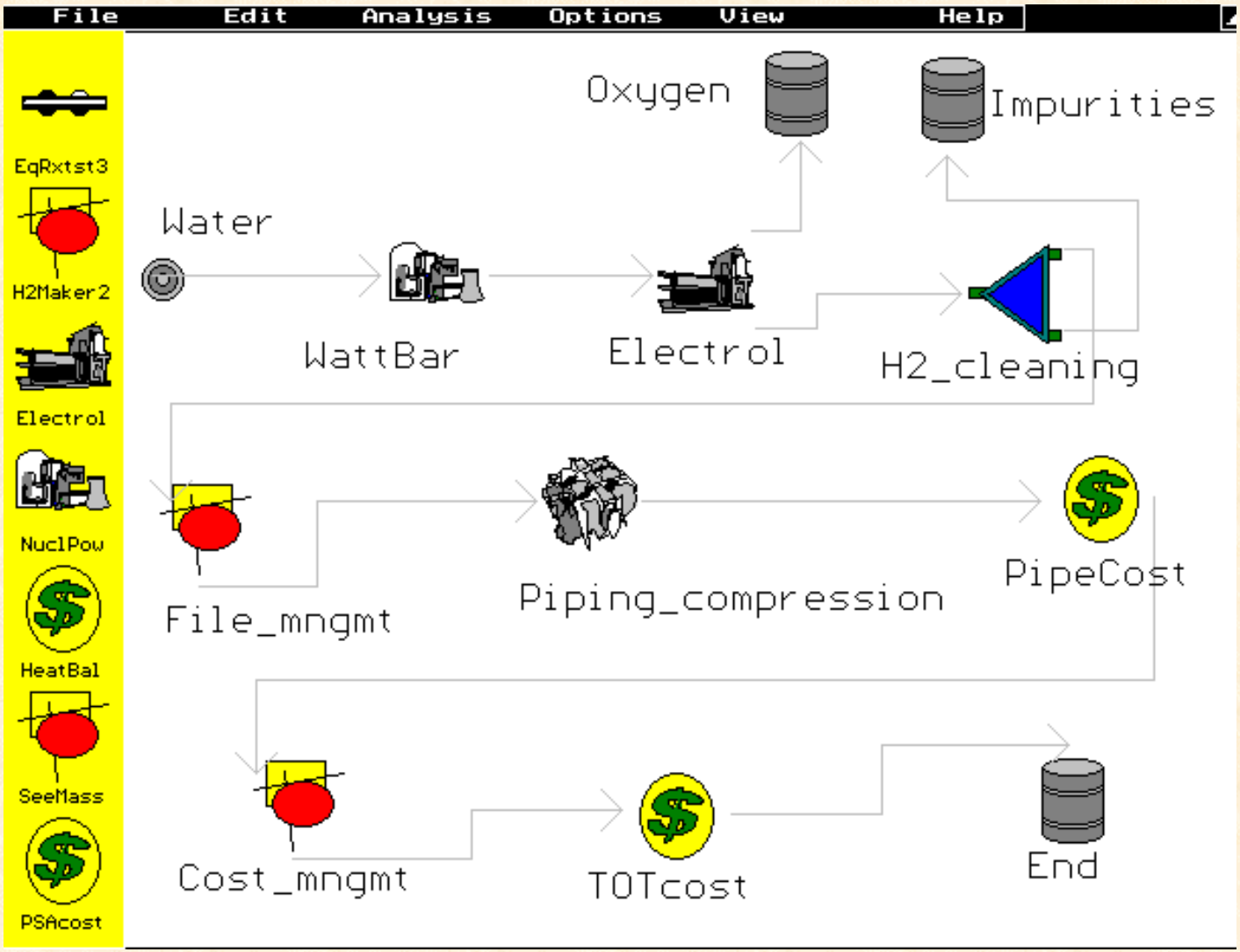
Production Cost

Analysis of H_2 production using TVA off- peak power

OAK RIDGE NATIONAL LABORATORY
U. S. DEPARTMENT OF ENERGY

UT-BATTELLE

FLOW Representation of TVA case



Skill Set – Models that include H_2 (continued)

- ***H_2 System including Thermochemical Cycles (U_3O_8, NaOH, and H_2O)***
  - ***2004***
  - ***System integrates process stages***
  - ***Models are based on thermodynamic, heuristics, and mass and energy balance.***
  - ***Model platform FLOW accessing HSC5 equilibrium models.***
  - ***Limitations: Does not have large thermodynamic databases, but may import from other programs***

Skill Set – Models that could be adapted

- ***Previous model for mixed waste treatment evaluation that used multicriteria methodology (technical risk, cost, reliability, availability, maintainability, etc.) can be adapted for the H_2 Economy***
  - ***FLOW was used for every scenario analyzed***
  - ***Models are based on thermodynamics and unit operations***
  - ***Model platform was FLOW***
  - ***FLOW does not have an extensive thermodynamic database but can import information from other sources***

Skill Set – Capabilities Summary

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

Studies

- ***Significant past studies that relate to hydrogen***
  - *H_2 Production System using Electrolysis with TVA Off-peak Power*
  - *H_2 Production using Reforming and Shifting*
- ***Significant past studies that could be adapted to hydrogen***
  - *Mixed Waste Technology Selection Analysis*
- ***List current/planned hydrogen studies***
  - *Hydrogen Production Using a Novel Thermochemical Cycle*

Future

Plans/commitments from our Organization

Our Organization is providing:

- ***University students are being sponsored at ORNL to participate in various assignments to build relationships and to assess their future employment potential***
- ***Seed money is being used to further enhance and develop H_2 analysis capabilities***

David Greene Backup Slides

Skill Set - People

- ***Sujit Das – advanced vehicle technology simulation and cost analysis***
- ***David L. Greene – vehicle choice, fuel demand, transportation demand, policy analysis***
- ***Jerry Hadder – refinery modeling and analysis (retiring 2004)***
- ***Paul N. Leiby – dynamic non-linear modeling of economic systems, SPR optimization***
- ***Marc Melaina – (U. Mich.) fuel retailing, consumer behavior***
- ***Jonathan Rubin – (U. Maine) economic models, policy analysis***
- ***Rekha Pillai – operations research, supply chain analysis***
- ***Elzbieta Tworek – StrataG, infrastructure & supply chain analysis***
- ***I.G. Harrison, S.C. Davis, I.K. Busch, M.R. Hilliard, F. Southworth, B.E. Peterson, S.M. Chin, O. Franzese, ORNL***

Skill Set – Capabilities Summary

(Refer to H_2 Analysis Types – last Slide)

TYPE OF ANALYSIS	RESIDENT CAPABILITY?	STUDIES SPECIFIC TO H_2?	MODELS SPECIFIC TO H_2?
Resource Analysis	***Oil, conventional and unconventional***	***No***	***No***
Technoeconomic Analysis	***For advanced vehicles***	***Yes, for advanced vehicles***	***Yes, for fuel cell and IC H2 vehicles***
Environmental Analysis	***Yes or No***	***Yes or No***	***No***
Delivery Analysis	***Yes, supply chain logistics***	***Yes or No***	***Yes***
Infrastructure Development Analysis	***Yes (e.g., ORNIM)***	***Yes or No***	***Yes***
Energy Market Analysis	***Yes***	***Yes or No***	***Yes***

Materials Modeling Work Supports FreedomCAR

Focuses on the economic viability of advanced vehicle designs under consideration for light-duty vehicles by DOE/FreedomCAR

Analytical tools developed to examine the cost-effectiveness of new technologies both from component specific as well as system perspectives:

- Work done in collaboration with the industry partners and other national labs
- Component level cost and technical targets of FreedomCAR need to be met to achieve affordability of advanced technology vehicles. Carbon fiber polymer composites still remain a long term solution towards vehicle lightweighting.
- Lightweight body materials and advanced engine designs include some of the major research areas

ORNL has been a leader in Freight Transportation Research:

1) GeoFreight GIS/Bottleneck Analysis Tool (US Dept. of Transportation)

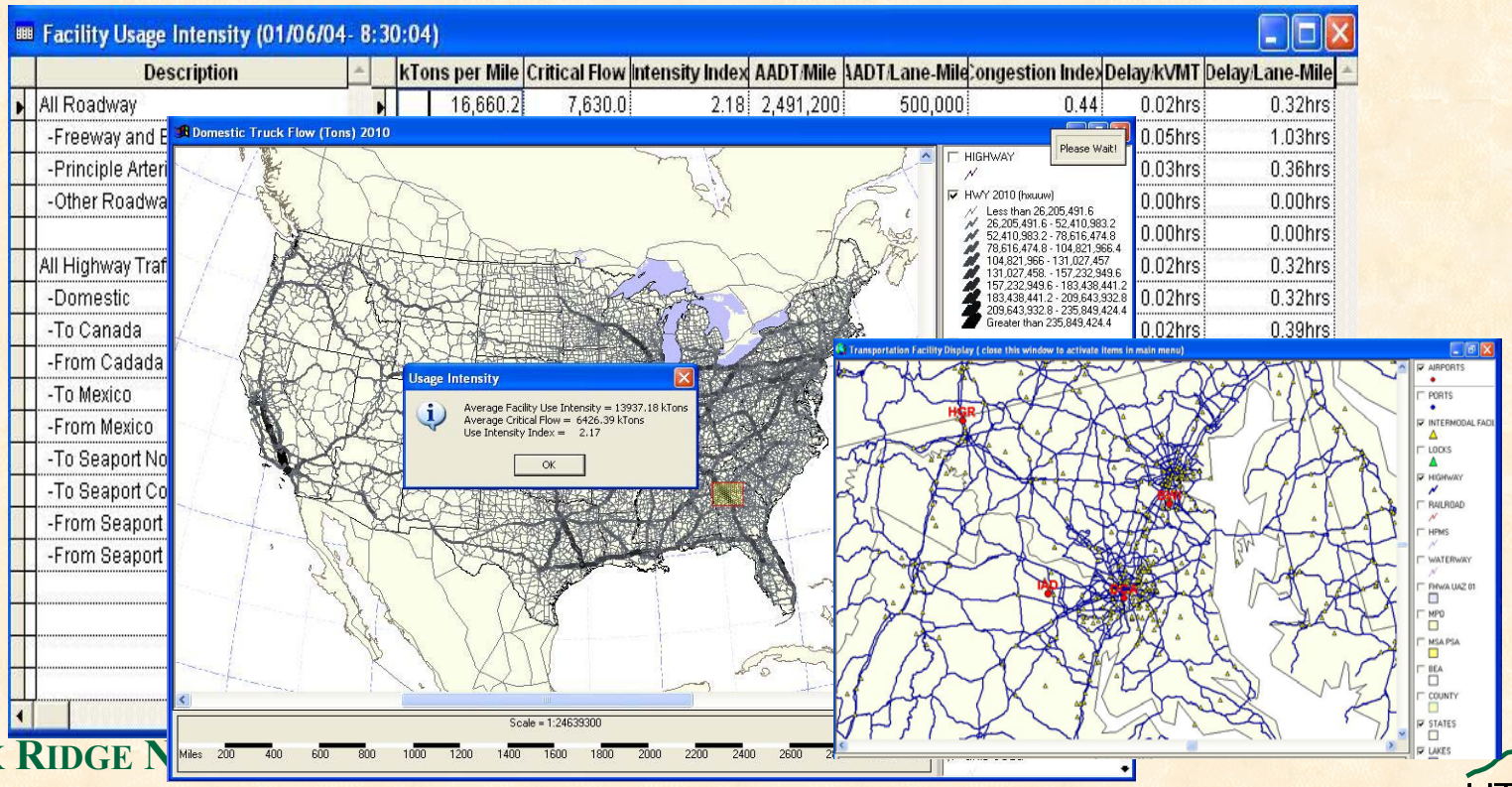
2) 2002 Commodity Flow Survey: Inter-modal Shipment Routing Models (US Dept. of Transportation)

3) Enterprise Model of Dynamic freight Supply Chains (National Science Foundation)

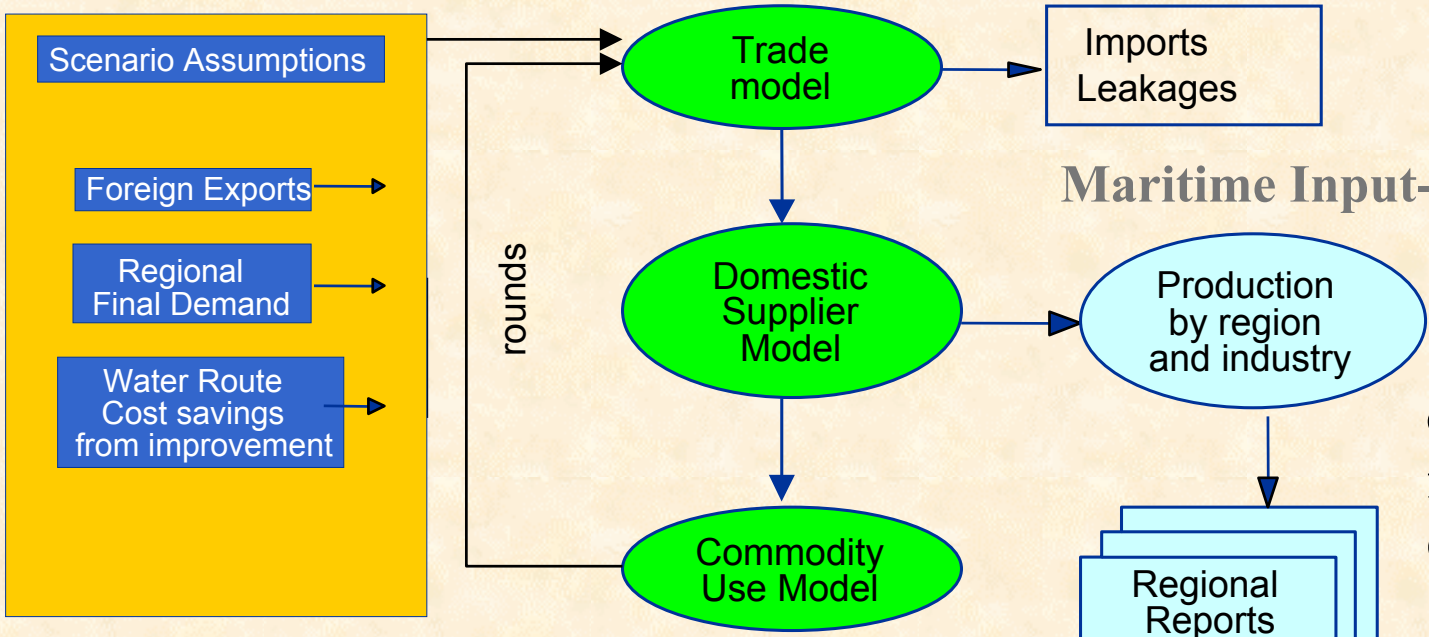
4) Maritime Input-Output Model for North America (US Army Corps of Engineers)

GeoFreight allows flexible area-based analysis of the multi-modal traffic and freight tonnage passing through a user-defined region (e.g. part of an urban area, a seaport).

This includes the ability to identify those origin-destination pairs of places impacted by traffic passing through the freight handling facilities in the area – on a nationwide basis.

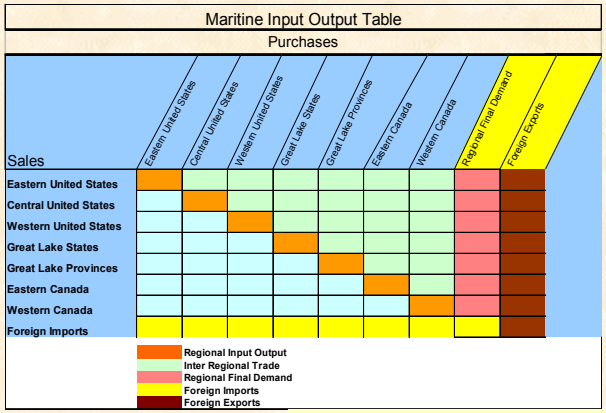


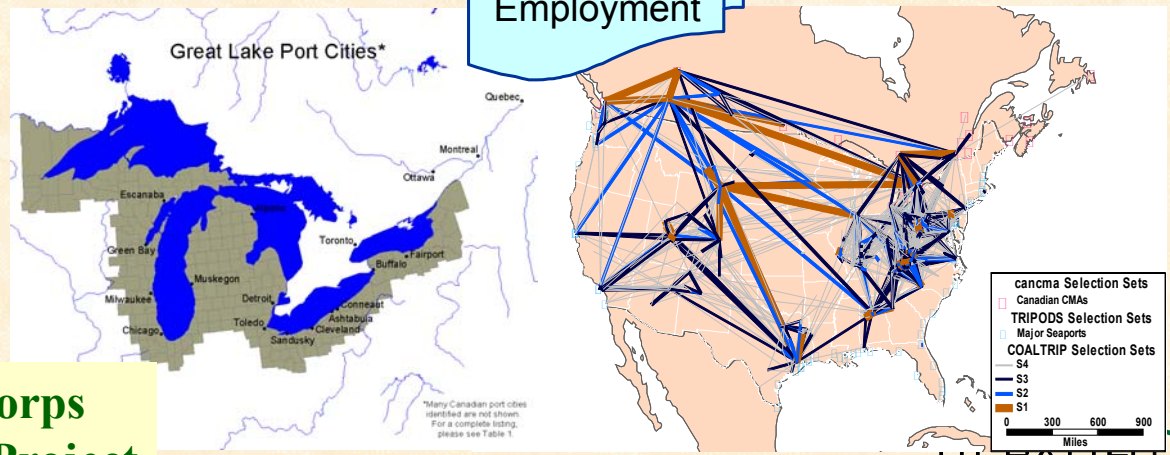
Estimating the economic impacts of improved waterway access for the Great Lakes/St. Lawrence Seaway



Maritime Input-Output Model

county-to-county freight flows, 60 commodities





OAK RIDGE NA
U. S. DEPARTMEN

US Army Corps of Engineers Project

UT-BATTELLE

Simulating US Freight Movements in the 2002 Commodity Flow Survey





National Highway Network Database

National Rail Network Database

Operational Rail Network Database

National Waterway Network Database

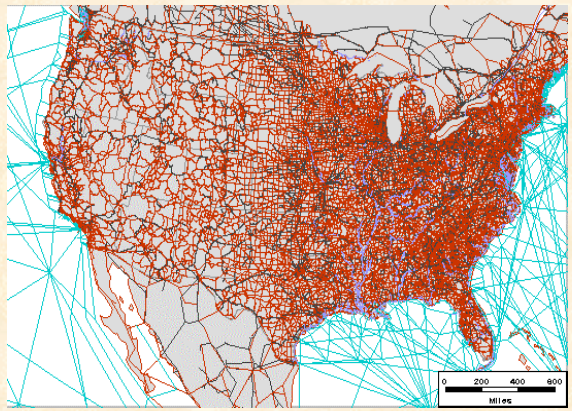
Operational Waterways Network Database

Global Seaways Network Database

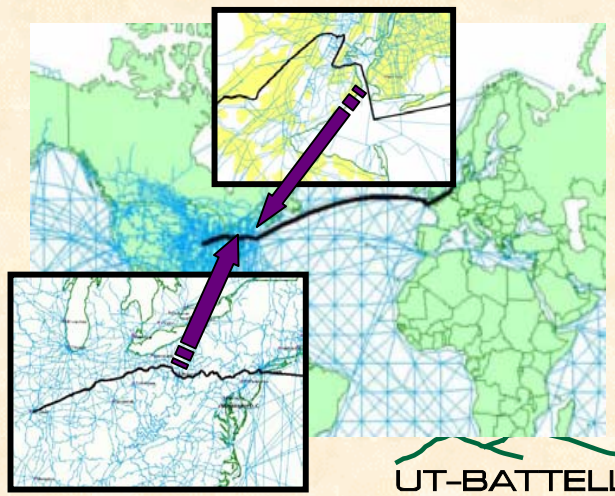
Intermodal, Truck, and Ports Terminals Databases

Combines Inland , Coastal, Great Lakes & Trans-Oceanic Links

CFS Unified Multimodal/Intermodal Freight Network



Project for the Bureau of Transportation Statistics, US DOT

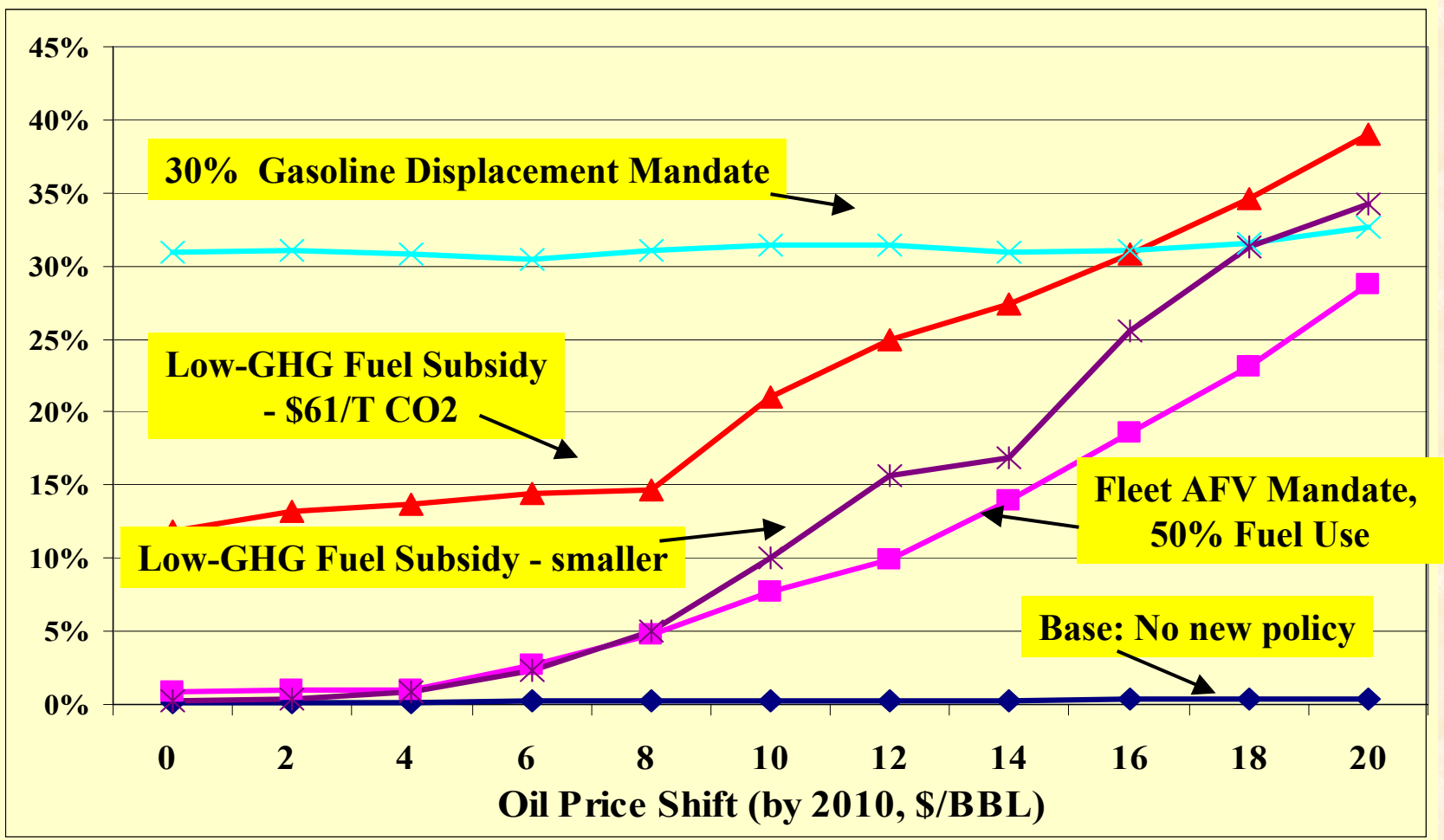


2.7 million zip –to-zip and US to foreign destination, single and multi-modal freight shipment routings
Based on ORNL multimodal freight networks

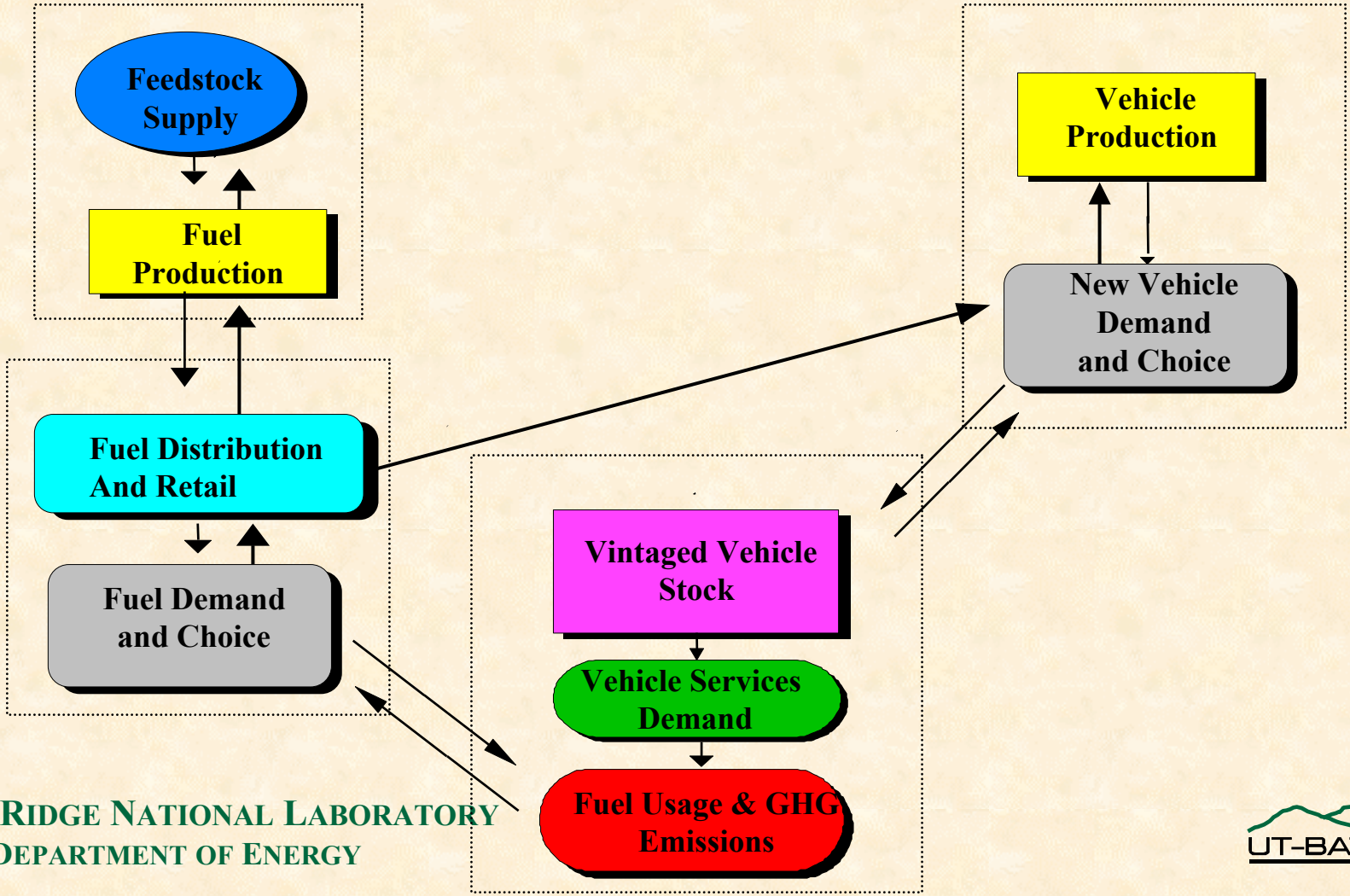
TAFV

TAFV Project Explored Effectiveness of Policy Tools at Different Oil Price Levels

Alternative Fuel Share in 2010 (%)



HyTrans finds a simultaneous solution that integrates consumer, fuel producer, fuel distributor and vehicle manufacturer decisions.

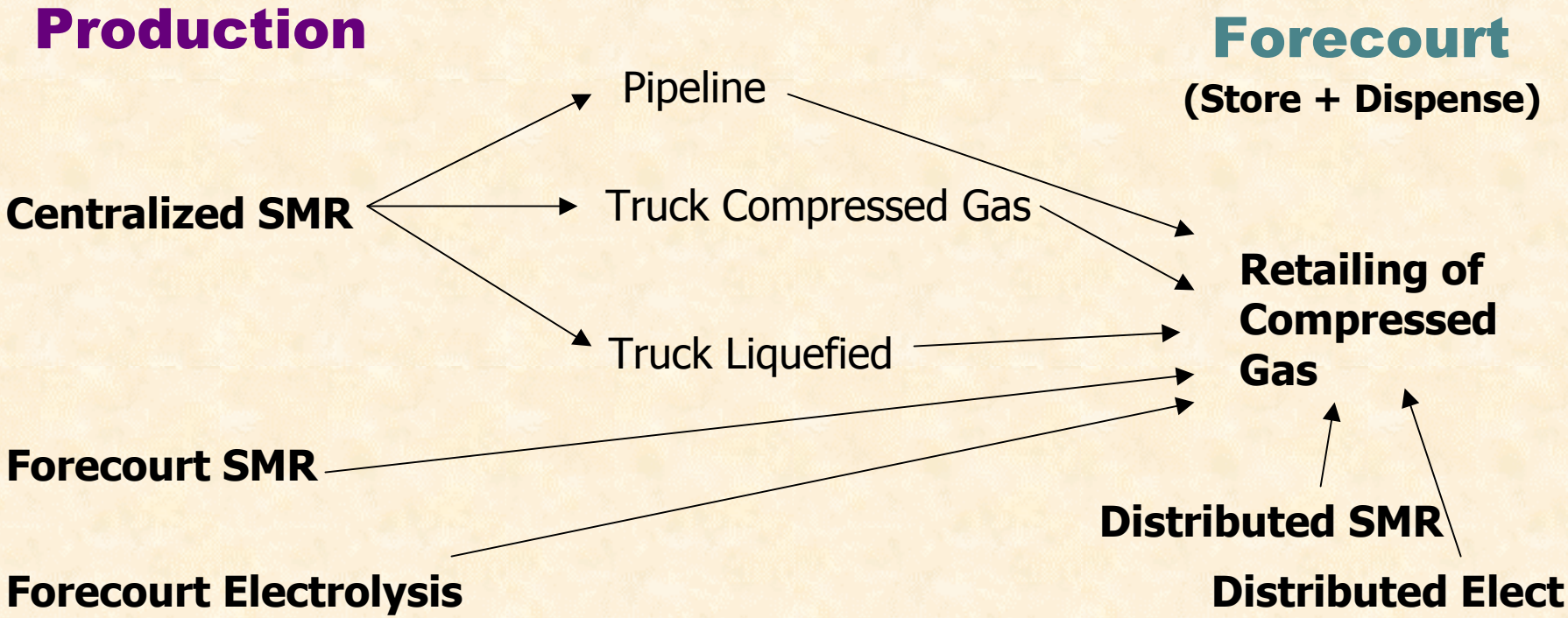


Delivery Mode Choice

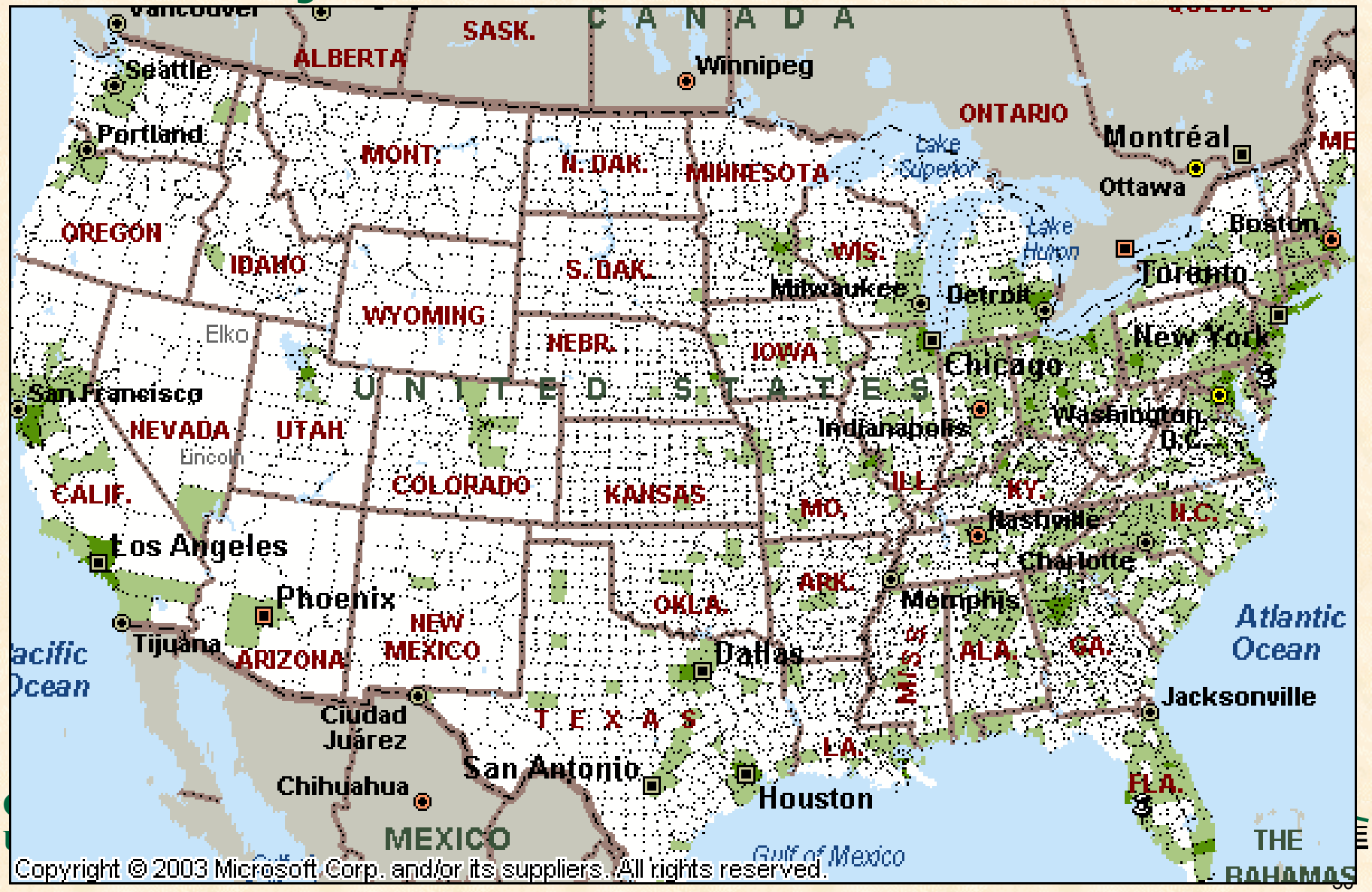
Will Depend on Distances, Demand Density, and Demand Volume

Delivery

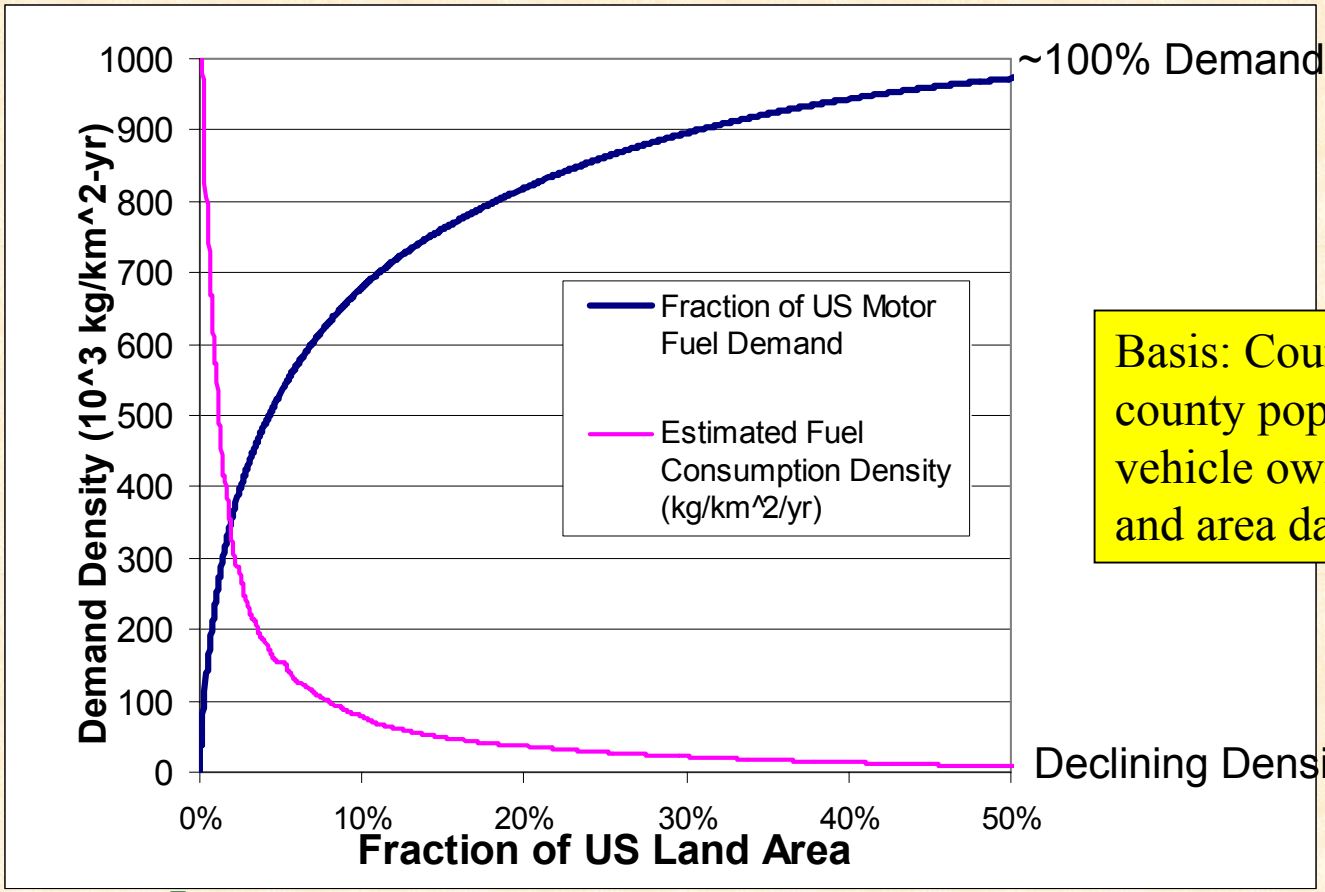
Includes: Compression/Liquefaction+Storage+Dispensing+ Transporting+Storage+Compression/Vaporization



A key factor in infrastructure evolution will be the density of motor fuel demand. In HyTrans there are three markets.

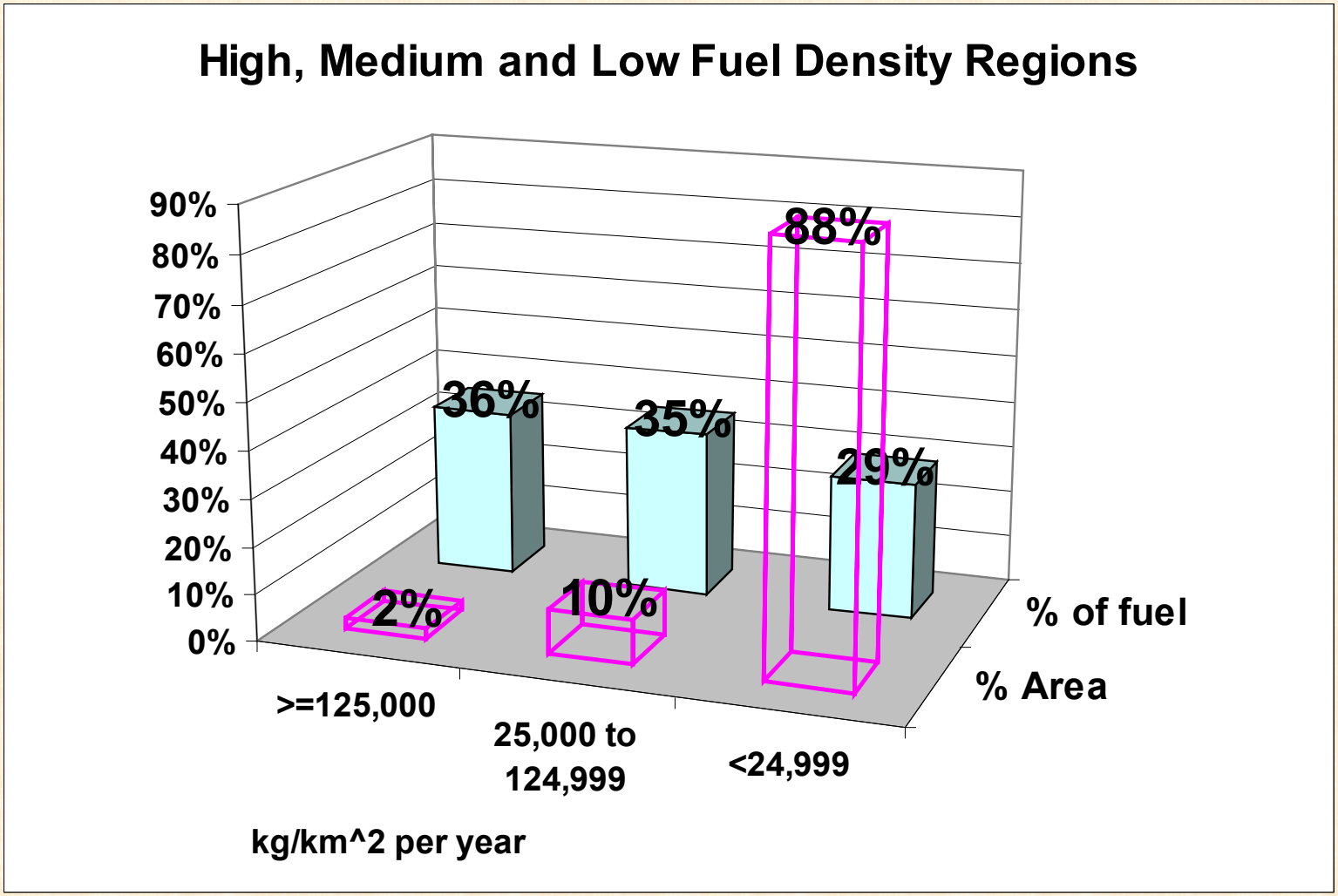


Most of US Area is Low Demand Density, But Med-High Density Areas Comprise Bulk of Motor Fuel Demand

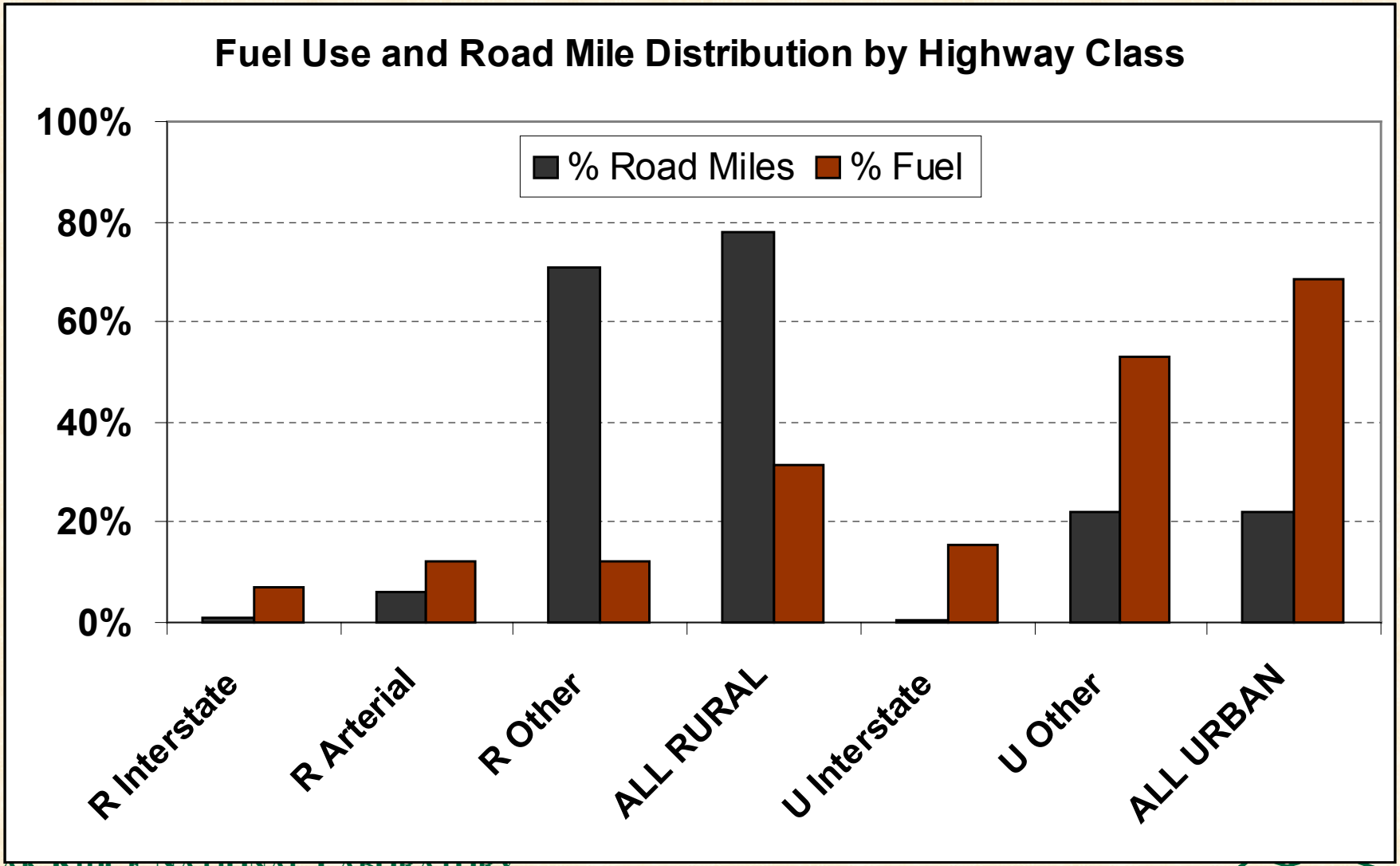


Basis: County-by-county population, vehicle ownership, and area dataset

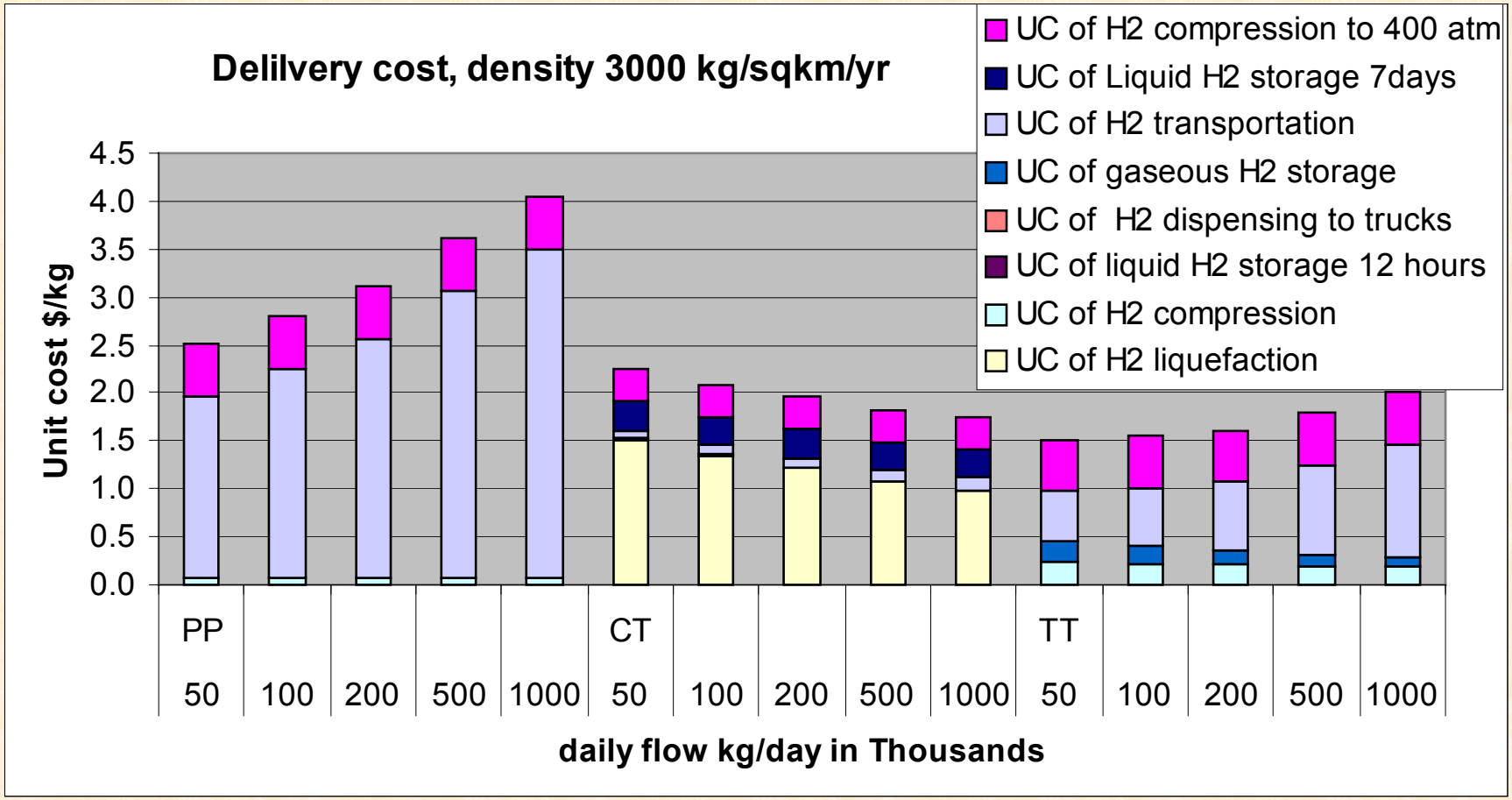
Most light-duty vehicle fuel is consumed in counties comprising about 10% of the land area of the US.



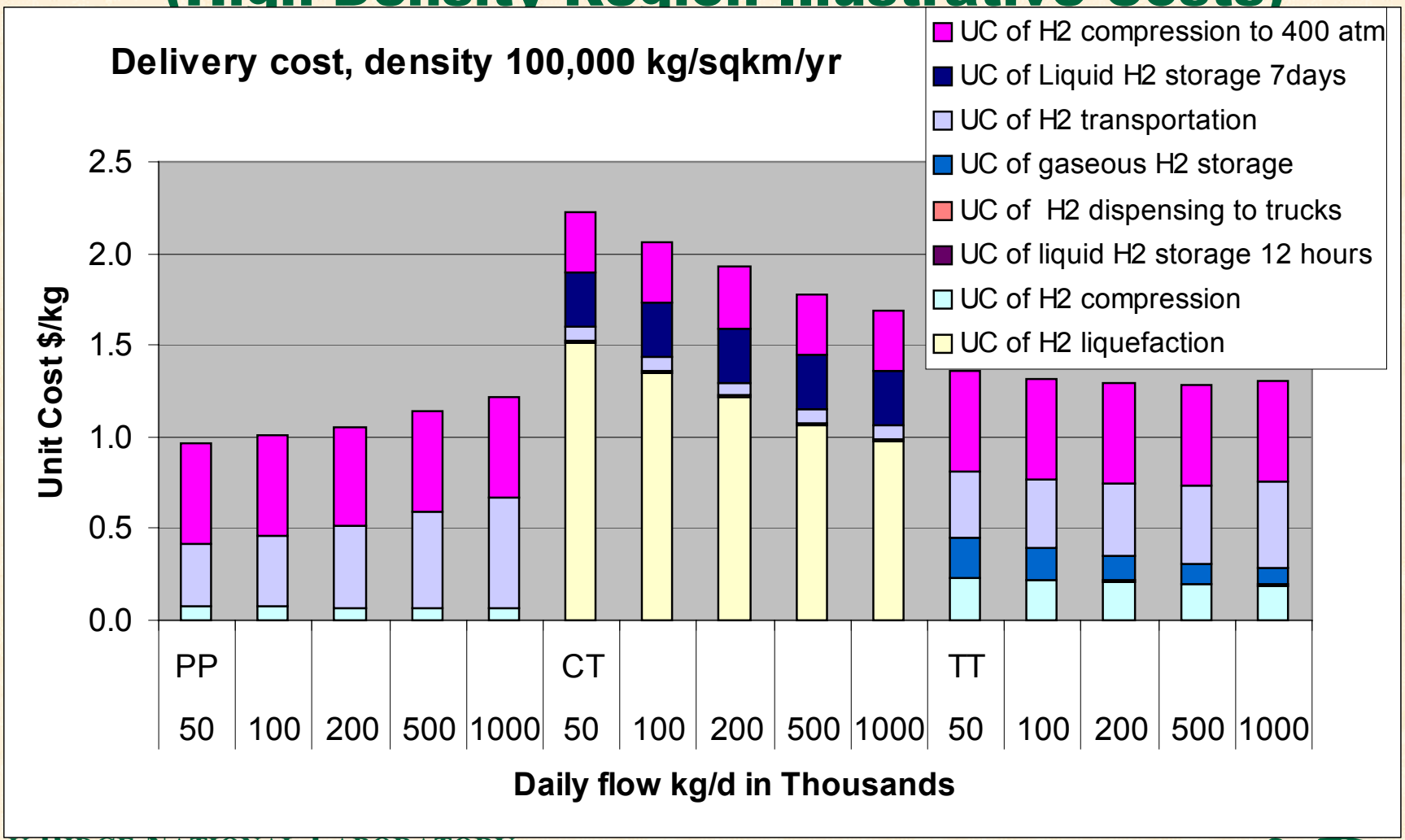
Thinking of highways as linear markets, most *rural* fuel is consumed on interstates and principal arterials.



Delivery costs depend on both production *scale* and *density* of demand. (Low Density Region Illustrative Costs)



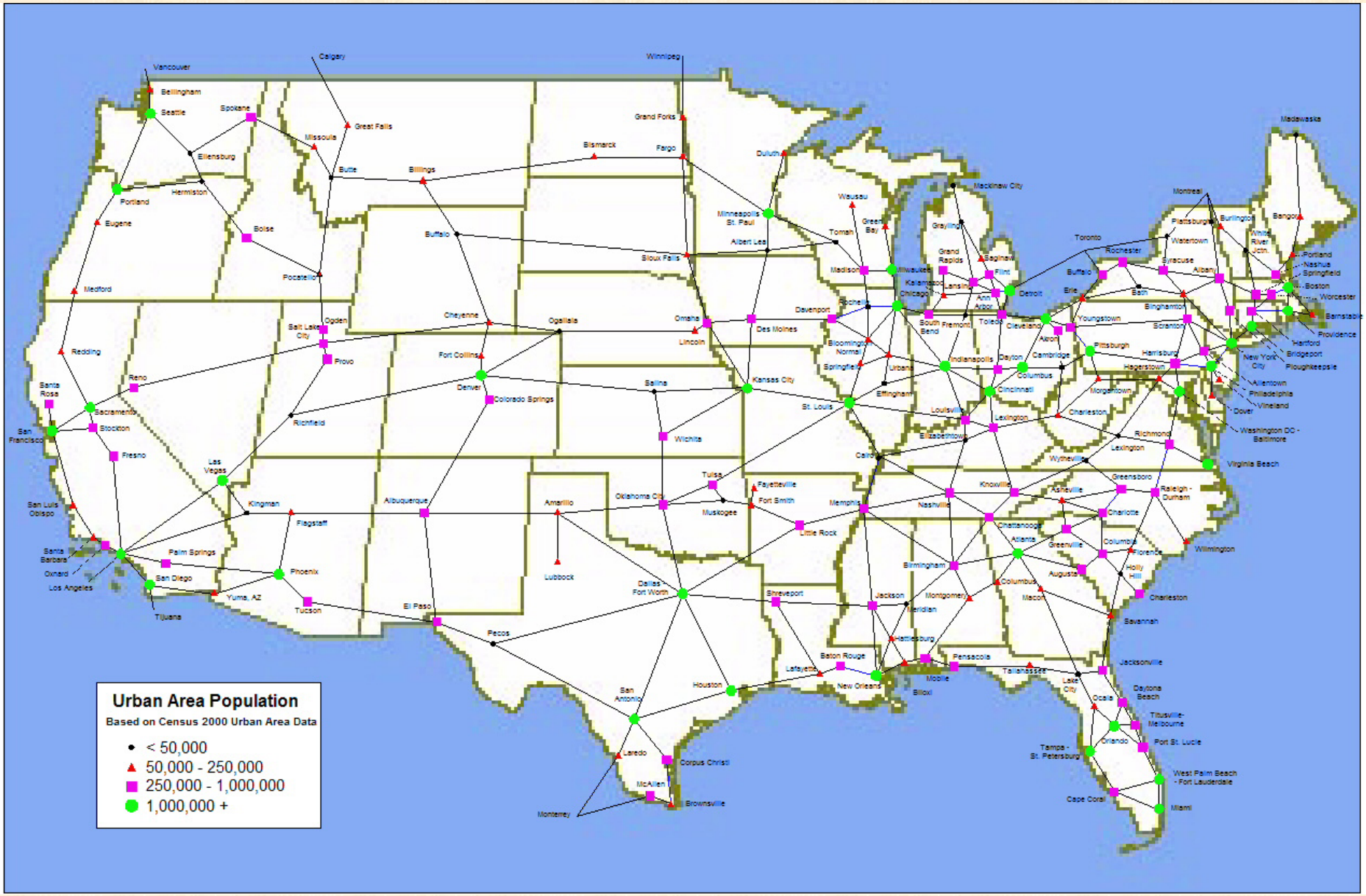
At high densities, pipelines do appear to dominate, but many questions remain. (High Density Region Illustrative Costs)



Improving our representation of fuel availability value to vehicle owner, via spatially explicit analysis (side-studies)

- UC Davis using urban models to measuring increased trip distance and travel time for limited local availability.
- The value of availability in non-local markets and other regions needs a rigorous logical framework.
- Availability in linear markets needs a rigorous formulation. Marc Melaina (U. Mich) addressing.

Spatial/GIS Approach to Availability Cost: Urban Area/Interstate Network Model



Hard problems remain for demand modeling:

- How to determine the value of availability in other regions?
  - Own region
  - Intercity
  - Other regions
- How to explore the unique value of the hydrogen fuel cell vehicle?
- How to design the most competitive vehicles?