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Hydrogen Analysis with the Sandia ParaChoice model

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Sandia National Laboratories

SAND 2015-XXXX

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U.S. DEPARTMENT OF ENERGY

NNSA National Nuclear Security Administration

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Overview

Timeline

- Start date: FY15 Q1
- End date: Project continuation determined annually

Budget

- FY15 funding: $100K

Barriers

- Availability of alternative fuel and charging infrastructure
- Availability of AFVs and electric drive vehicles
- Constant advances in technology
- Uncertainty in vehicle choice models and projections

Partners

- Interactions / Collaborations:
  - Ford: Real World Driving Cycles
  - Toyota
  - American Gas Association
  - DOT
  - ANL, ORNL, NREL, Energetics

Project was **not** reviewed in previous Merit Reviews

ParaChoice Relevance/Objective: parametric analysis across factors that influence the vehicle, fuel, & infrastructure mix

- *Objective*: ParaChoice captures the **changes to the Light Duty Vehicle (LDV) stock through 2050** and its dynamic, economic relationship to fuels and energy sources

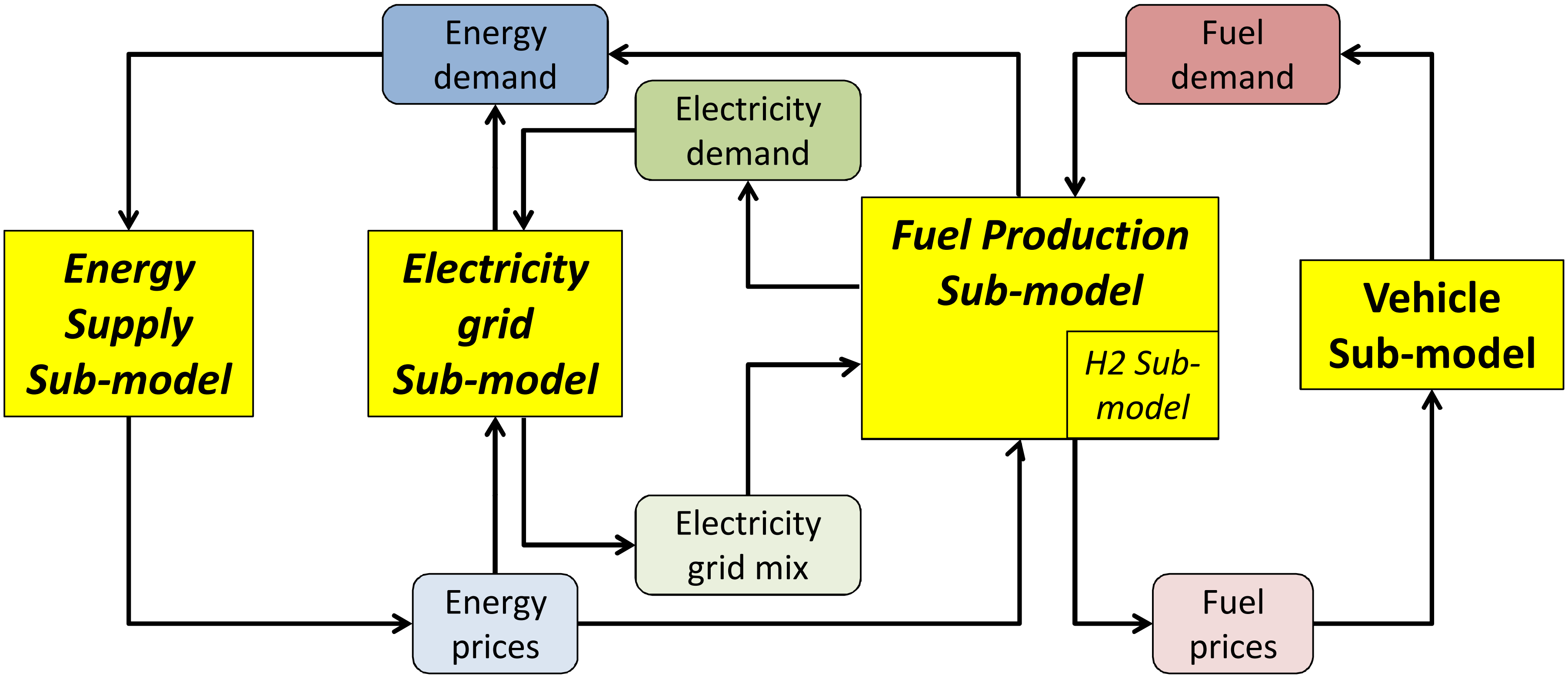
- *Uniqueness*: The model occupies an **system-level analysis layer with input from other DOE models** to explore the uncertainty and trade space (with 10,000s of model runs) that is not accessible in individual scenario-focused studies

- *Approach*: Model the **dynamics and competition** among LDV powertrains and fuels using **regional-level** feedback loops from vehicle use to energy source
  - Technologies are allowed to flourish or fail in the marketplace

- *Targets*: By conducting parametric analyses, we can identify:
  - The set of conditions that must be true to reach performance goals
  - Sensitivities and tradeoffs between technology investments, market incentives, and modeling uncertainty

- *Focus for FY15 FCTO funded work*: Add hydrogen production and fuel cell electric vehicles to existing Sandia ParaChoice model to further the FCTO mission
  - Determine how FCEVs compete in the fleet with conventional and other AEVs
  - Determine effects of FCEV and H2 adoption on Gasohol usage and GHG emissions
  - Evaluate choices in H2 production pathways and consequences for H2 pricing, FCEV adoption, and GHG emissions

Modeling Approach: The high-level model diagram depicts the feedback loop of energy supply<-->energy carrier<-->vehicle



Modeling Approach: The model has many segments to capture the different niches of LDV consumers

Vehicle Stock Segmentation

Powertrain
SI
SI Hybrid
SI PHEV10
SI PHEV40
CI
CI Hybrid
CI PHEV10
CI PHEV40
FCEV
E85 FFV
E85 FFV Hybrid
E85 FFV PHEV10
E85 FFV PHEV40
BEV75
BEV100
BEV150
BEV225
CNG
CNG Hybrid
CNG Bi-fuel

Housing type
- Single family home without NG
- Single family home with NG
- No access to home charging/fueling

VMT Segmentation

State
48 CONUS +
Washington, DC

Density
Urban
Suburban
Rural

Size
Compact
Midsize
Small SUV
Large SUV
Pickup

Age
0-46 years

Driver Intensity
High
Medium
Low

Geography
Vehicle
Demographics

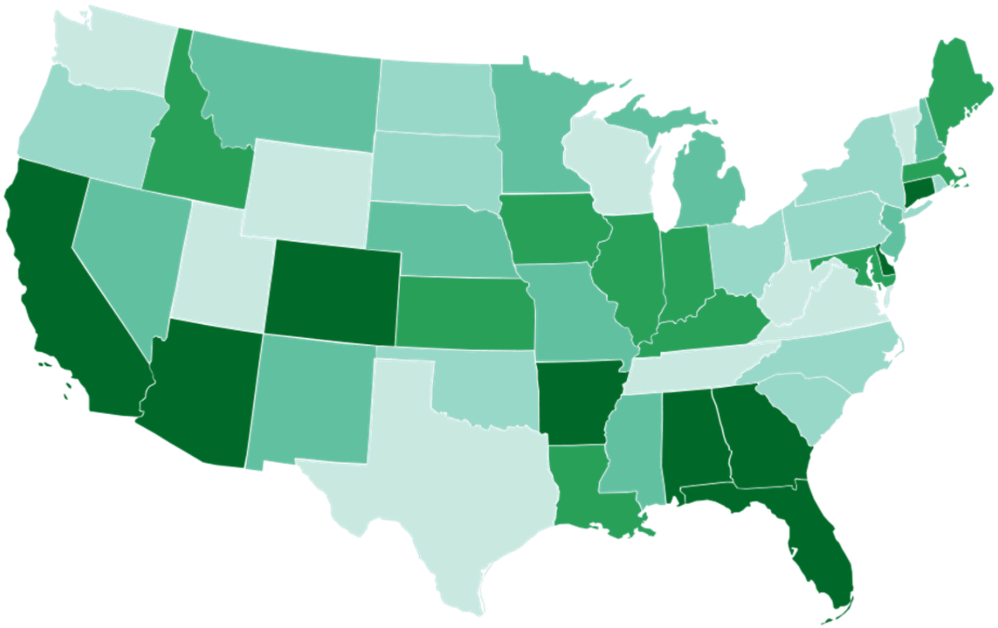
Fuels
Gasoline
Diesel
Biodiesel
Ethanol
Electricity
CNG
Hydrogen

Energy Sources
Petroleum
Natural Gas
Coal
Biomass
Solar/Wind

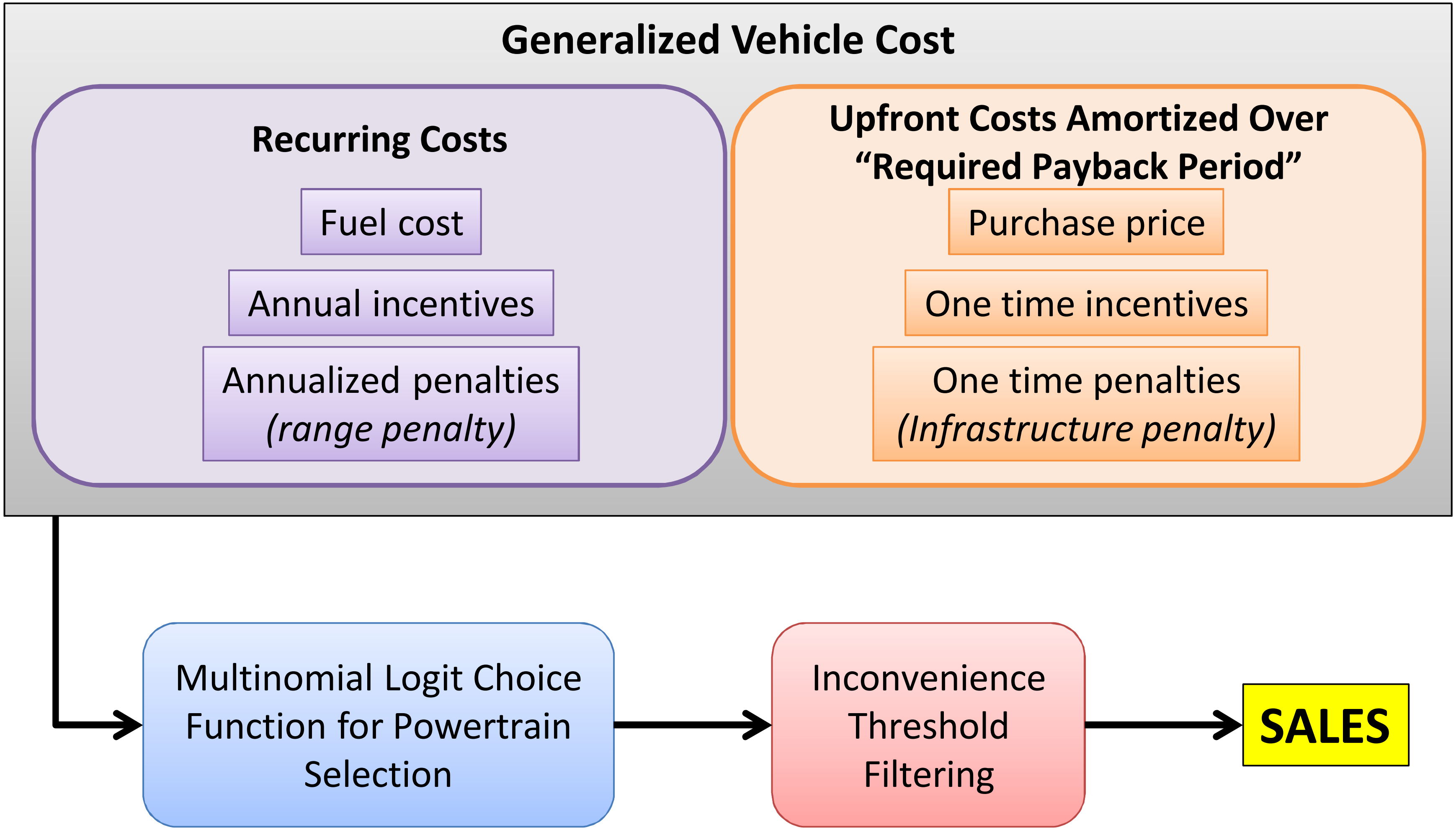
Modeling Approach: Energy supplies, fuels, and vehicle mixes vary by state

State-level Variations

- Vehicles
  - Numbers, sizes, drive-train mixes
- Driver demographics
  - VMT intensity, urban-suburban-rural divisions, single-family home rates
- Fuels
  - Costs, hydrogen production pathways, electricity mix, taxes & fees, alternative fuel infrastructure
- Energy supply curves (as appropriate)
  - Biomass, natural gas
- Policy
  - Consumer subsidies and incentives

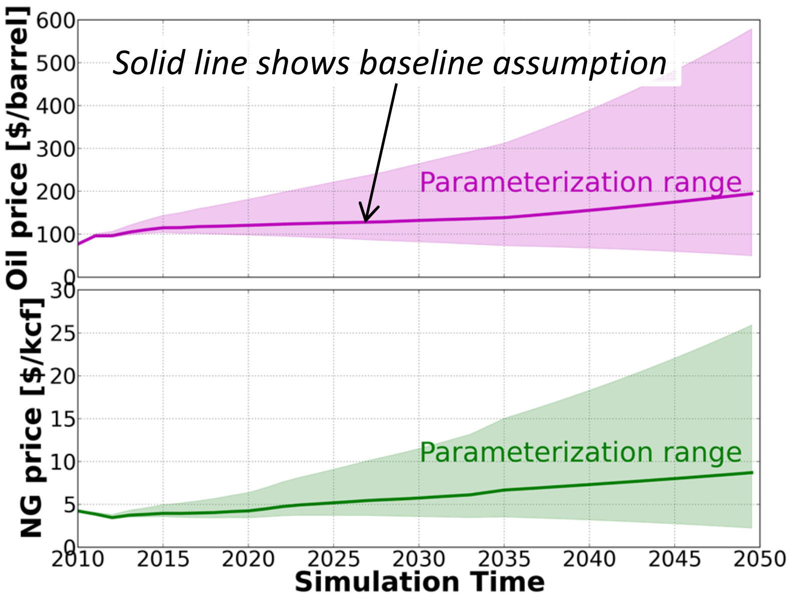


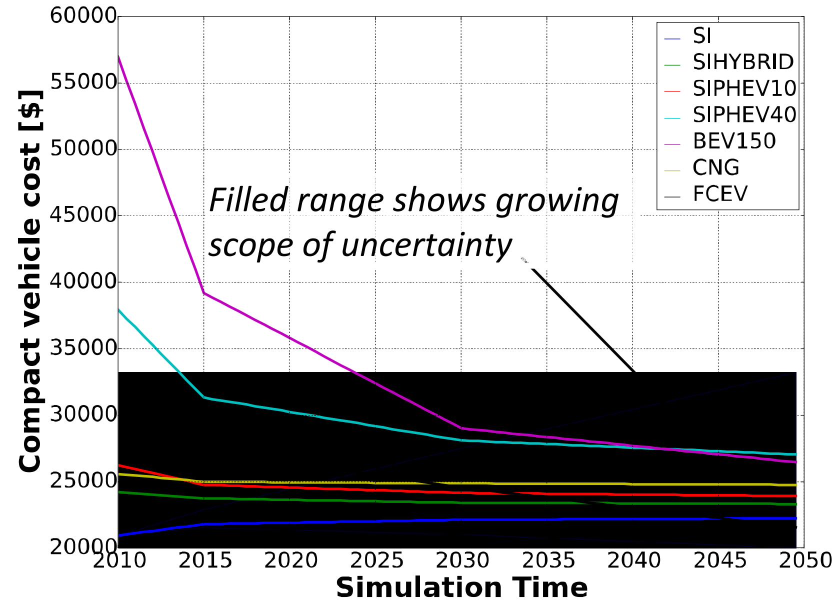
Modeling approach: A multinomial logit choice function assigns consumer purchase shares based on price sensitivity to a generalized cost



FCEV are treated the same as other AEVs

Approach: Parameterization helps account for uncertainty in commodity prices, technology performance, modeling assumptions, etc.

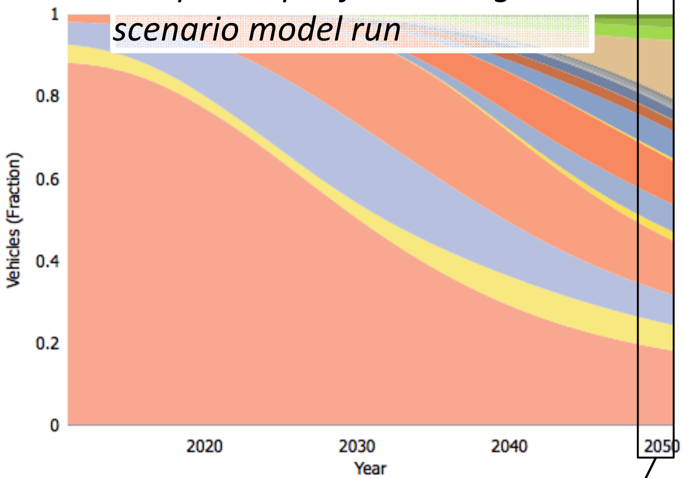




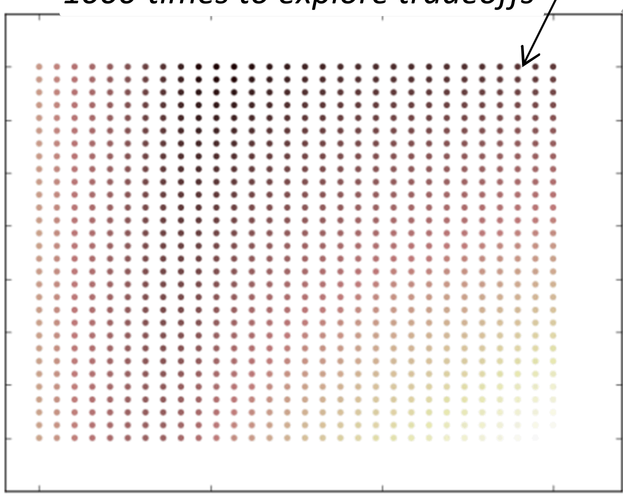
Uncertain costs shown for SIs only

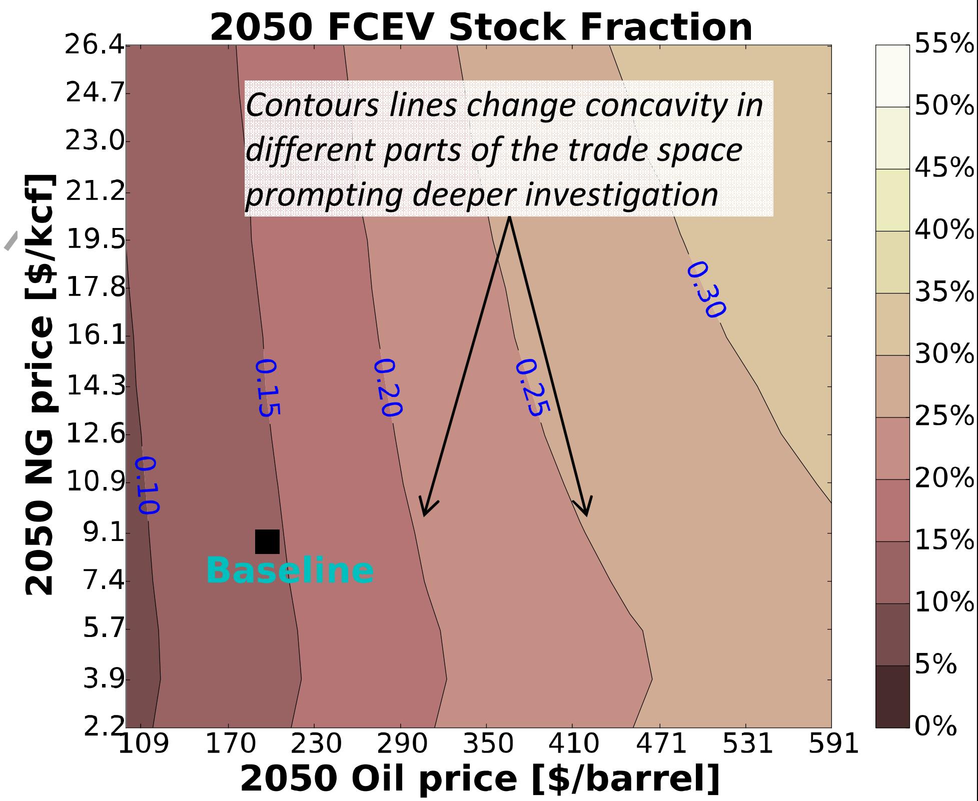
Approach: Parametric studies focus on one, two, and all parameter variations to explore the trade space

Sample output from a single-scenario model run



Parameter space is sampled 1000 times to explore tradeoffs





Contours lines change concavity in different parts of the trade space prompting deeper investigation

Tradeoff between price uncertainty and market incentives

Contour features reveal trade-space insights

Approach: Progress vs. Milestones

Completed

- Added hydrogen production pathways and refueling to ParaChoice model
  - Industrial
  - Distributed SMR
  - Distributed Electrolysis
  - Central SMR
  - Central Coal
  - Central Electrolysis
  - Central SMR + sequestration
  - Central Coal + sequestration
- Added FCEVs to vehicle submodel
- Initial verification testing completed, e.g.,
  - Verified that model matches Macro System Model reported costs
  - Compared model outputs to other published or modeled results as appropriate (e.g., GREET)

Ongoing

- Analysis of FCEV adoption, H2 production pathways, and sensitivity analysis
- ~ 1 month ahead of schedule

Project was **not** reviewed in previous Merit Reviews

Accomplishments and Progress: Summary of H2 fuel production logic added to the ParaChoice model

Init:

- Number of H2 stations is taken from AFDC (~50 nationally, ~20 in CA)
- No pre-existing dedicated H2 production capacity
- H2 prices are assumed to be industrial prices at lowest volume pricing, obtained from Hydrogen and Fuel Cells US Market Report, 2010
- FCEV technology costs from *Autonomie* 2011

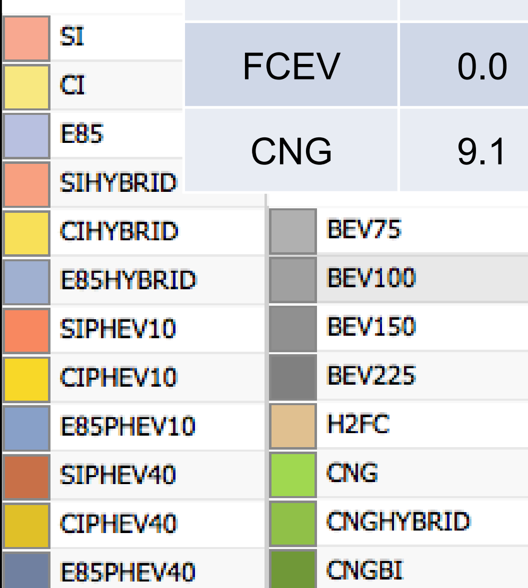
Loop:

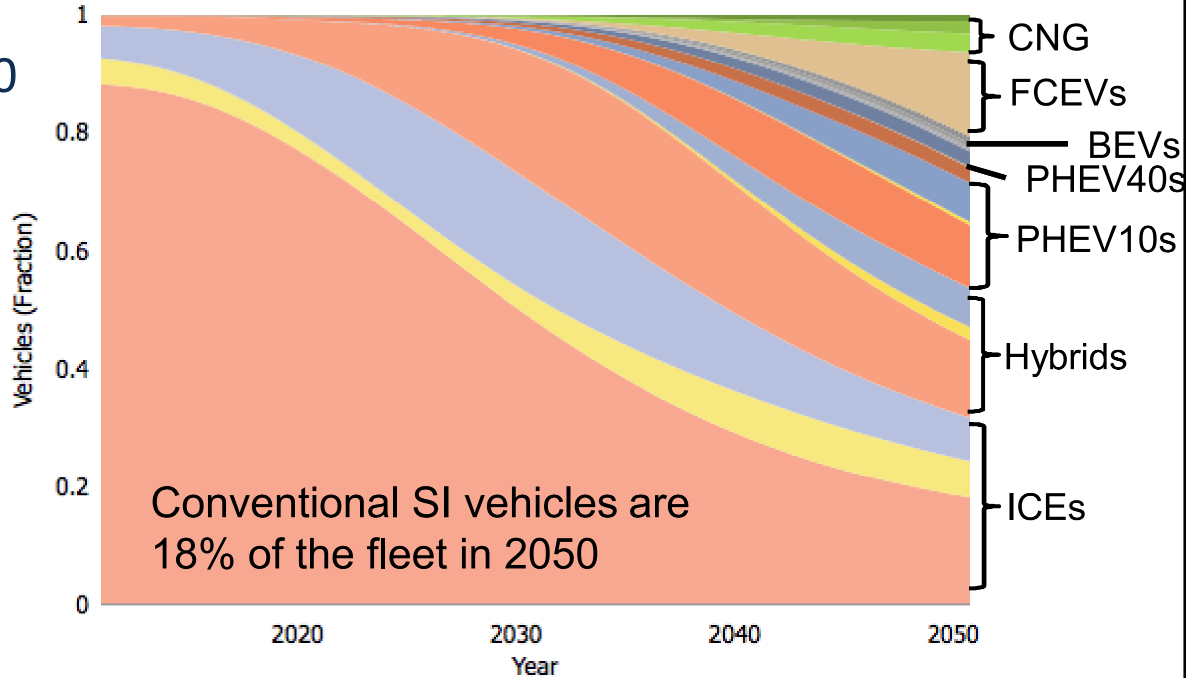
- Fleet sets new H2 demand
- By state, if H2 demand > existing capacity: choose between
  - Industrial H2- chosen at very low demand if no dedicated capacity exists
  - Dedicated distributed production
    - Full station capacity is 1,500kg/day (H2A)
    - Prices are scaled up when usage < capacity
  - Dedicated central production
    - Full station capacity is 50,000kg/day (H2A)
    - Only an option if rate of demand increase is at least 12,500 kg/day/year (compliant with H2A assumption of 50,000kg/day plant capacity, 40 year lifespan, and 90% production capacity)
- Retire old production capacity
- New H2 prices are supplied to vehicle sub-model to compute new FCEV sales
- Refueling stations and assoc. penalties are updated based on new FCEV market share

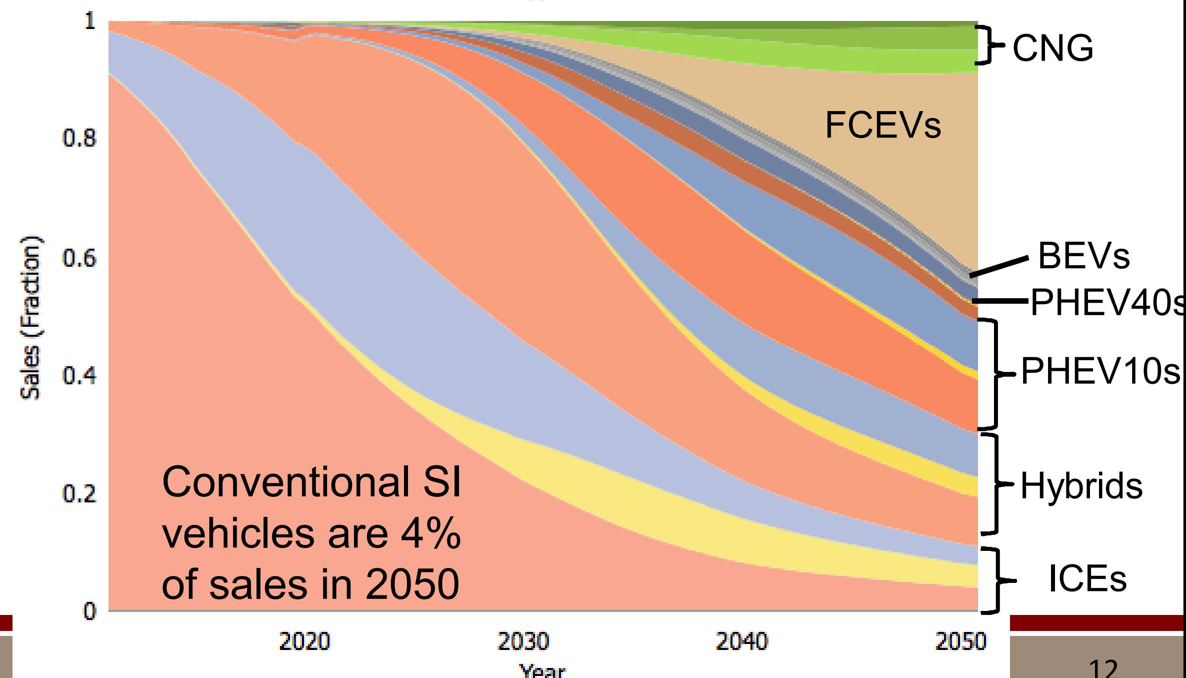
Key Results:

FCEVs have a potential for significant fleet share in 2050

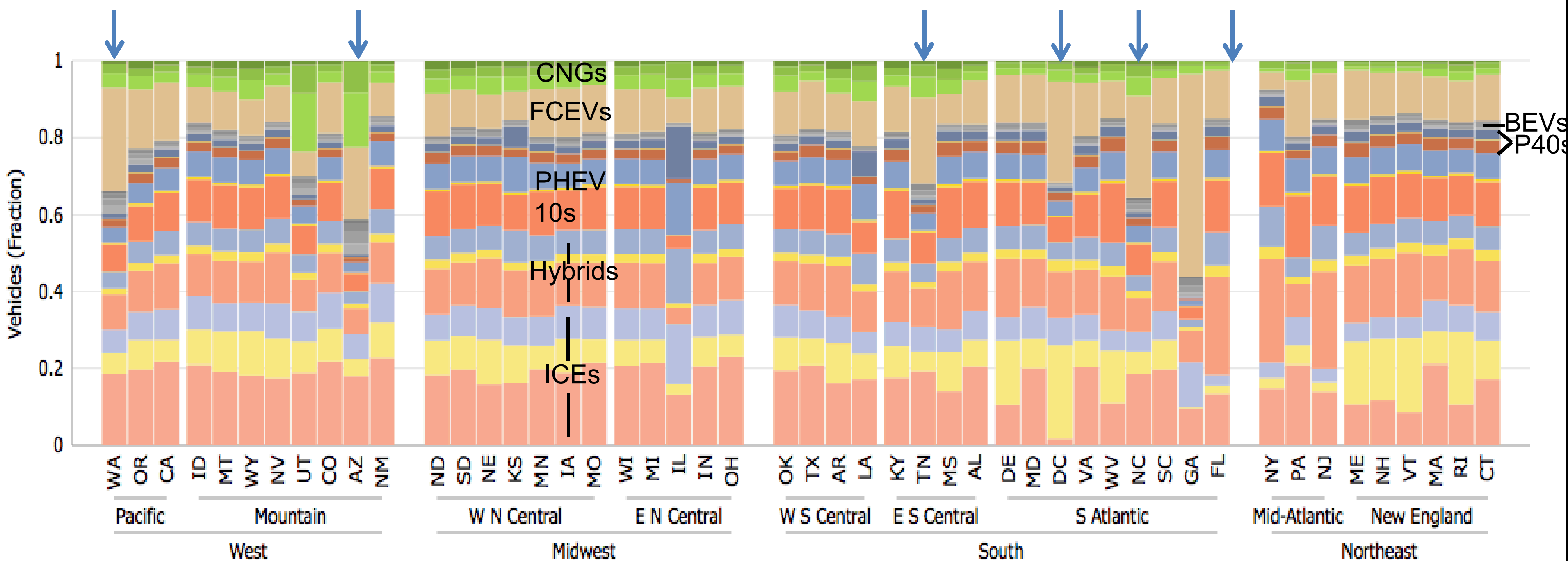
Power-train	% 2050 fleet	
	No FCEV	FCEV
ICE	34.2	31.8
Hybrid	25.8	21.9
PHEV10	21.6	17.9
PHEV40	6.1	5.3
BEV	3.2	2.5
FCEV	0.0	14.3
CNG	9.1	6.4



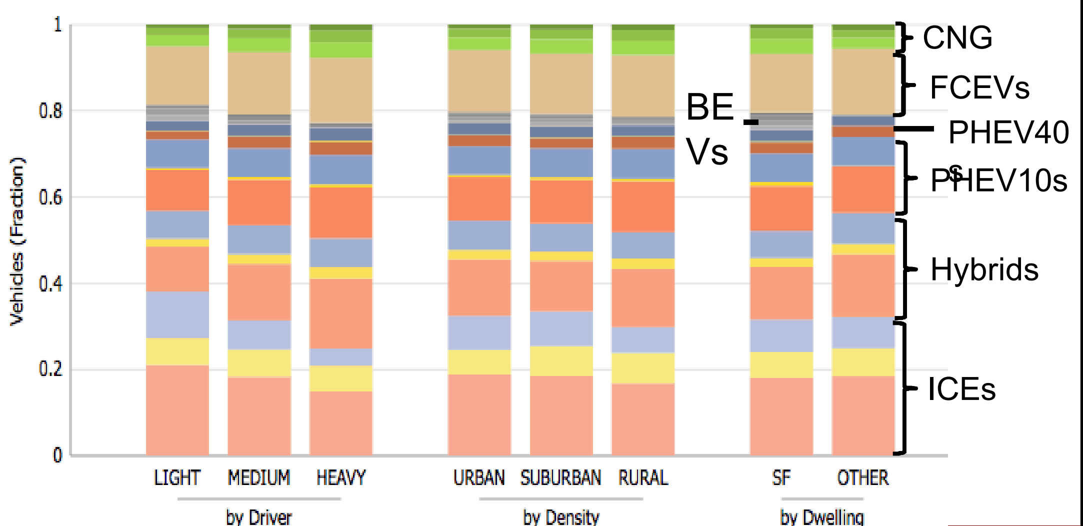




2050 fleet breakdown by region and population segment



State	FCEV motivators
GA	Non-sunsetting $5000 tax credit
NC	HOV worth $625/yr; H2 at $0.08/mi by 2029 (gas at $0.15/mi)
WA	Tax reduction; H2 at $0.08/mi by 2030 (gas at $0.16/mi)
DC	H2 at $0.09/mi by 2030 (gas at $0.21/mi)
TN	$2500 tax credit for first 1k vehicles; HOV
AZ	Tax reduction, HOV



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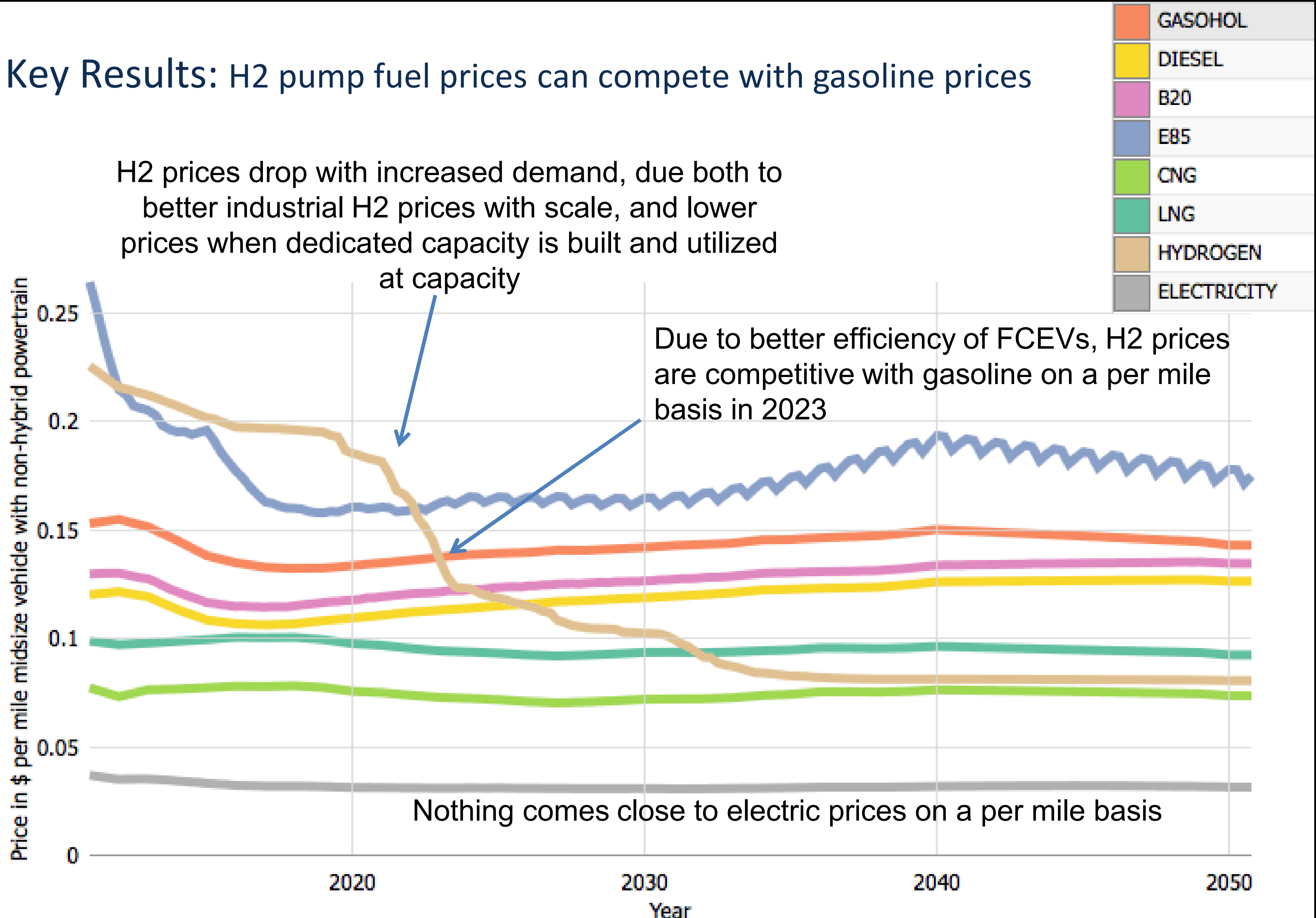
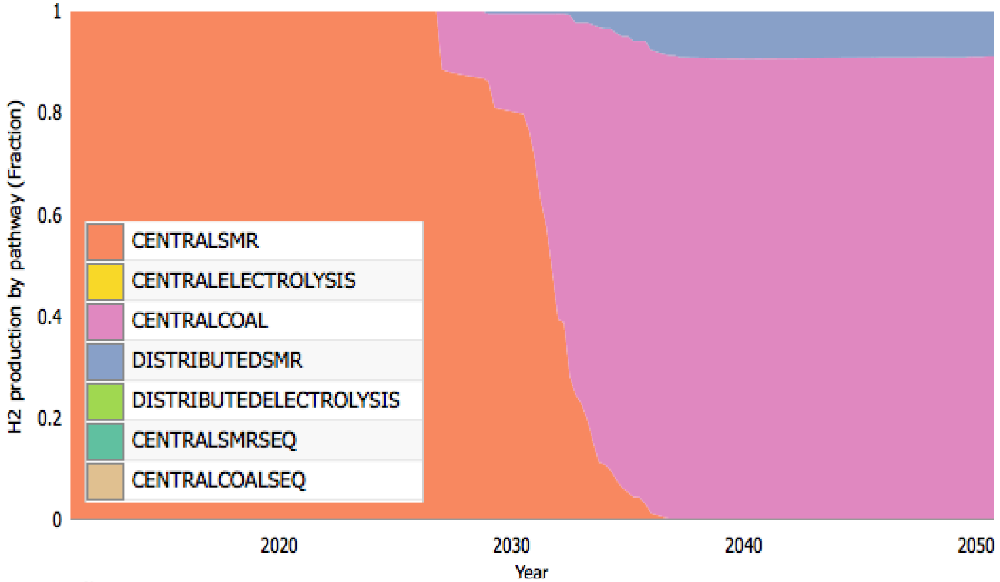
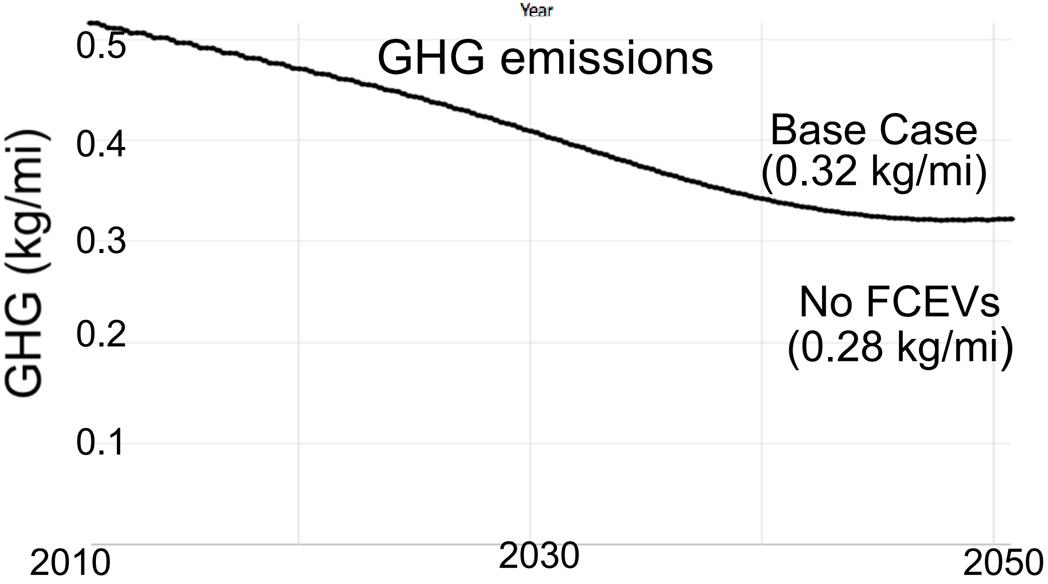
Key Results: H2 pump fuel prices can compete with gasoline prices



Key Results: Market driven production pathway mix increases GHG emissions



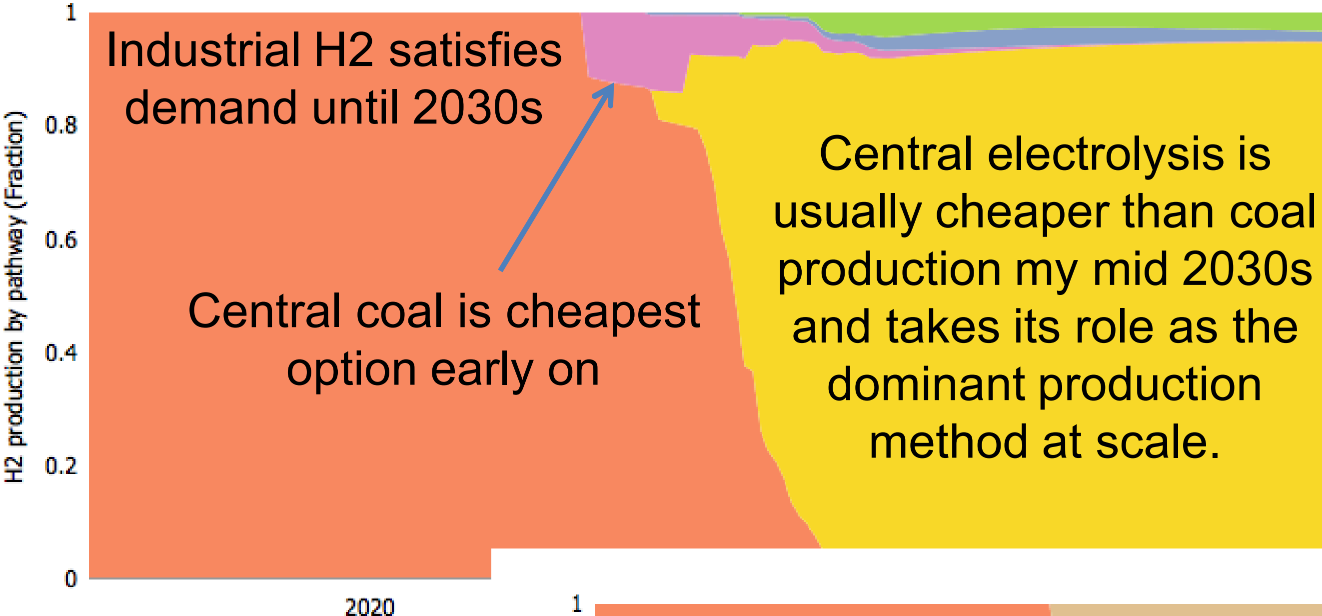
Most refueling stations rely on industrial H2 until the early 2030s. When vehicle demand makes the dedicated production options economical, central coal and distributed SMR become the dominant production pathways.



The prevalence of coal in H2 production actually leads to an increase of GHG emissions over a fleet without FCEVs.

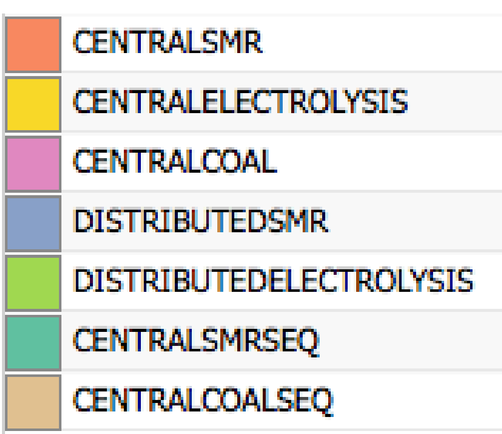
Production pathway mix: Scenario of low cost electrolysis:

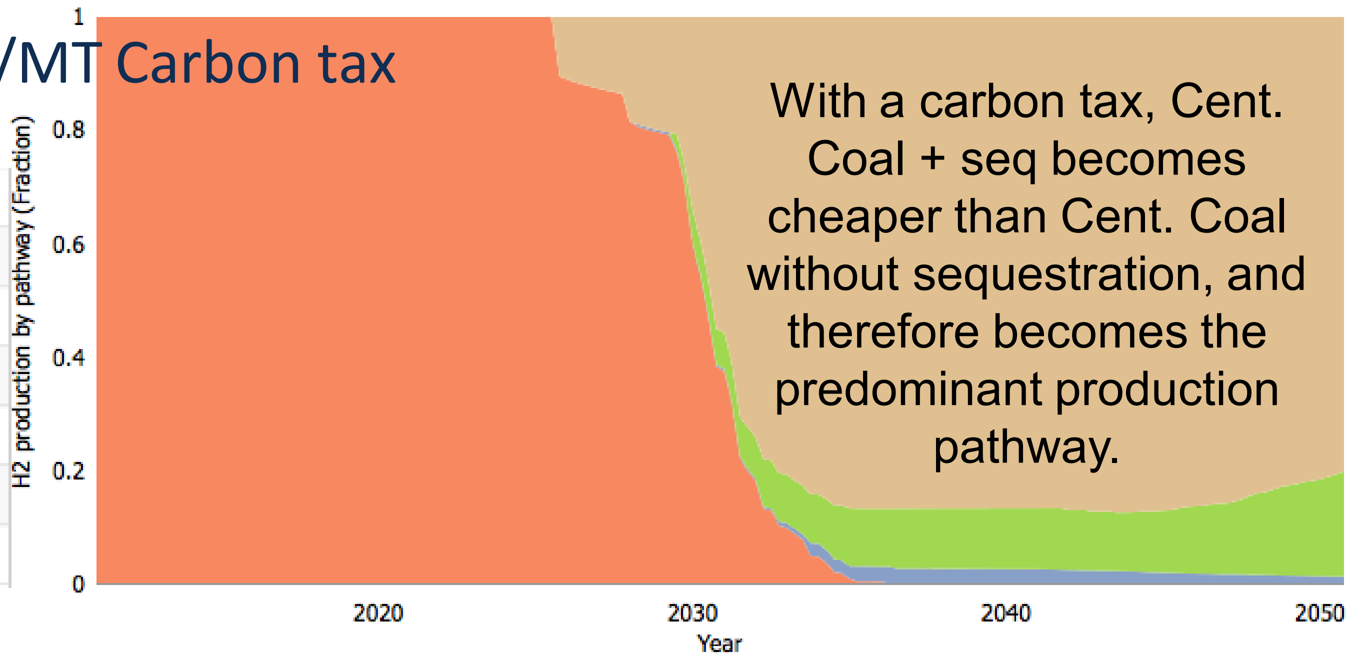
($3.50/kg by 2015)



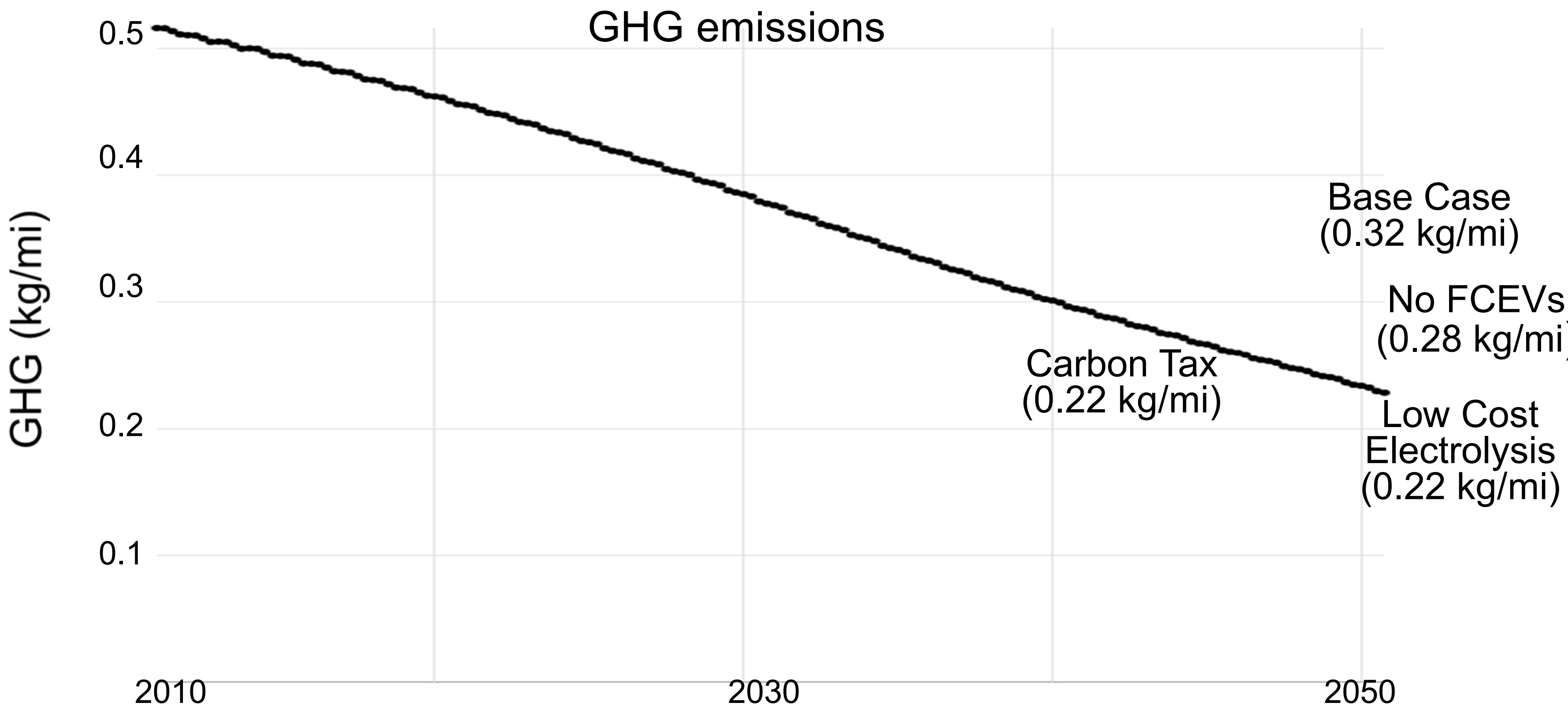
Key Results: There are ways to get around the GHG emission increase

Scenario of $200/MT Carbon tax



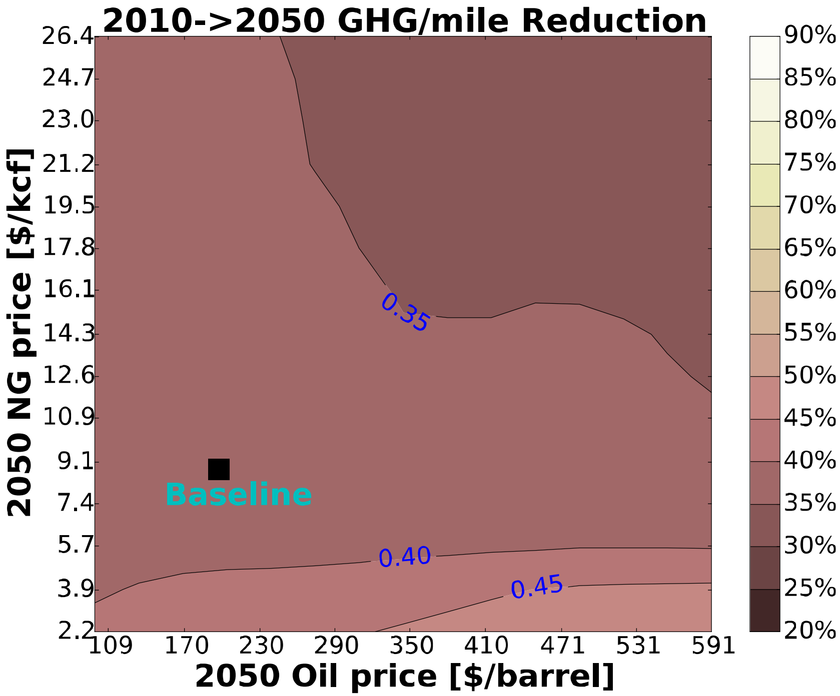


Key Results: The inclusion of FCEVs in the market place does not necessitate an increase in GHG emissions.



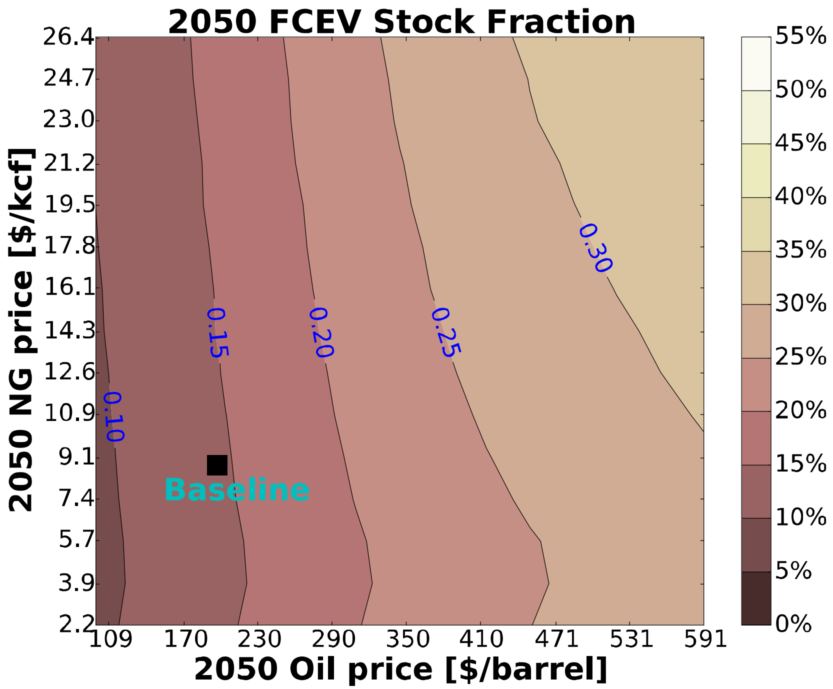
A $200/MT Carbon tax will achieve the same 2050 GHG emissions as inexpensive ($3.50/kg) H2 from electrolysis, but produces a steeper decline to that level. Low cost electrolysis incentivizes clean H2 production pathways and increases FCEV adoption. A carbon tax increases FCEV adoption, shifts H2 production to lower carbon pathways, increases PHEV40 market shares, and increases non-petrol usage of all PHEVS and Bi-fuel vehicles. All of these lead to lower carbon output per mile.

Key Results: Parameterization allows us to explore the variables affecting PHEV adoption and GHG Emissions.



When both oil and NG are expensive, FCEVs become favorable in the market price. However, the cheapest production method is coal, driving GHG emissions up.

Low natural gas prices make CNG vehicles more economical, but also drive down prices of H2 produced via NG SMR, making FCEVs more economical. The competition between CNGs and FCEVs powered by H2 from coal and NG creates a complex dynamic for GHG emissions and FCEV adoption.



Collaboration with other institutions

- No funding given to other institutions on behalf of this work
- Technical critiques received from Ford Motor Company, General Electric, American Gas Association, and other conference engagements
- The underlying ParaChoice model has been developed using funding from a variety of sources
- Dawn Manley will be presenting VTO-funded ParaChoice analysis (project ID VAN014) on Thursday, June 11 at 11am

Proposed future work

- **Explore effects of:**
  - Mandated carbon sequestration for H2 production on FCEV adoption and GHG emissions
  - Fuel cell cost uncertainties on FCEV market adoption
  - 2015 H2 price (industrial H2 price markup) on FCEV adoption
- **Deliverables**
  - Parametric assessments of these factors that affect FCEV adoption, petrol reduction, and GHG emissions
  - Publications and conference presentations
  - Scenario comparison

Summary

- FCEVs and H2 fuel are now part of the Pathways ParaChoice model
- For base case parameters:
  - Hydrogen can play a large role in the 2050 fleet
  - Inclusion of FCEVs leads to a 15% reduction in gasoline consumption in 2050
  - However, due to relatively inexpensive hydrogen production via Cent. Coal, overall GHG emissions may increase when FCEVs are included in the market
- If technology improvements could drive the cost of electrolysis down to approximately $3.50 by 2050, 30% of the mileage driven by 2050 could be on hydrogen, and the average GHG emissions could drop by 0.1kg/mi
- A Carbon tax of $200/MT will also drive down GHG emissions, by increasing FCEV adoption, shifting H2 production to lower carbon pathways (sequestration), and increasing other alternative fuel use
- Parametric approach allows exploration of broad range of scenarios and tradeoffs
- Future work will expand on this analysis of the place of FCEVs in the vehicle fleet and on the pathways used to produce Hydrogen as a vehicle fuel

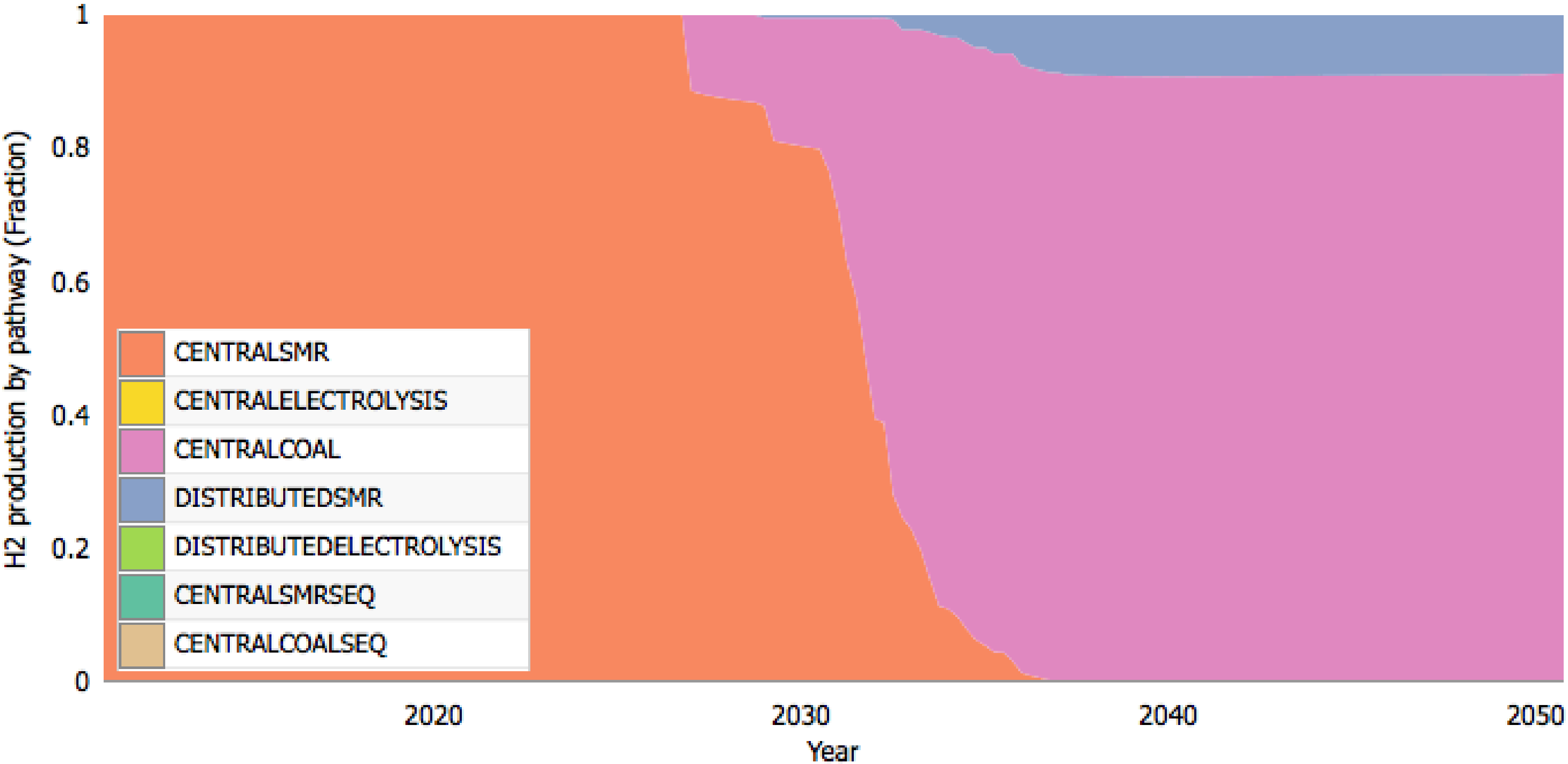
Technical Backup Slides

H2 pricing, production, and emissions assumptions and data sources

- Energy intensity and efficiency factors for the pathways come from the NREL-Sandia *Macro Systems Model*, which itself aggregates other DOE model inputs (e.g. H2A, HDSAM)
- Emissions factors for the pathways comes from *GREET* (latest version)
  - Fuel prices can be influenced by carbon taxes
- H2 pump fuel costs and GHG emissions by pathway are taken from MSM for 2015 technologies and efficiencies. These costs are divided into:
  - Production/transportation feedstock costs
  - Production electricity costs
  - State and federal taxes and fees
  - All other costs (e.g. fixed, O&M) associated with production, transport, and distribution

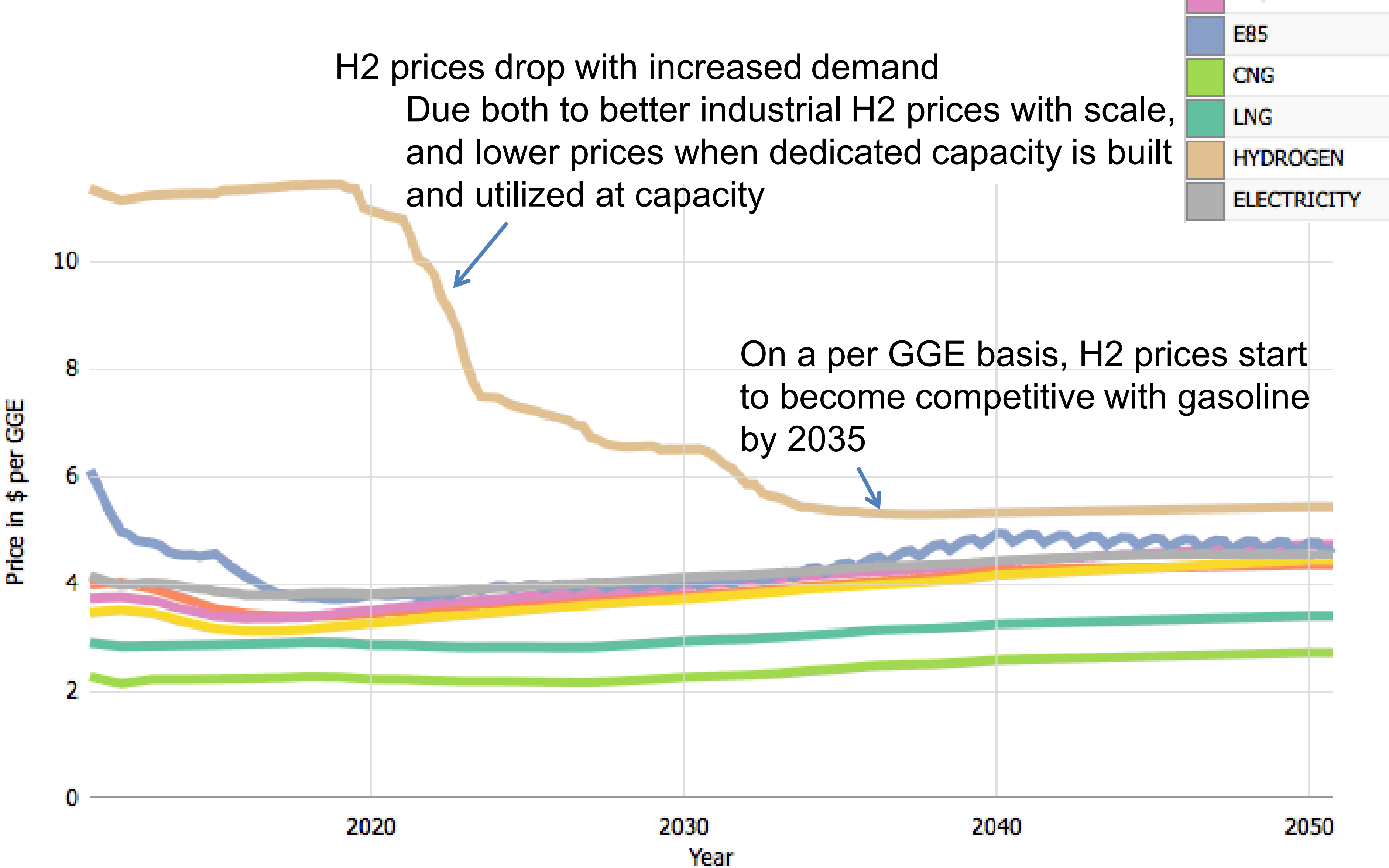
Pathway	Dist. SMR	Dist. Elec	Cent. Coal	Cent. SMR	Cent Elec.	Coal + Seq	SMR + Seq
Cost at scale (2007$)	4.59	6.61	4.58	5.17	7.51	5.15	5.39

Case 1: Production pathway mix

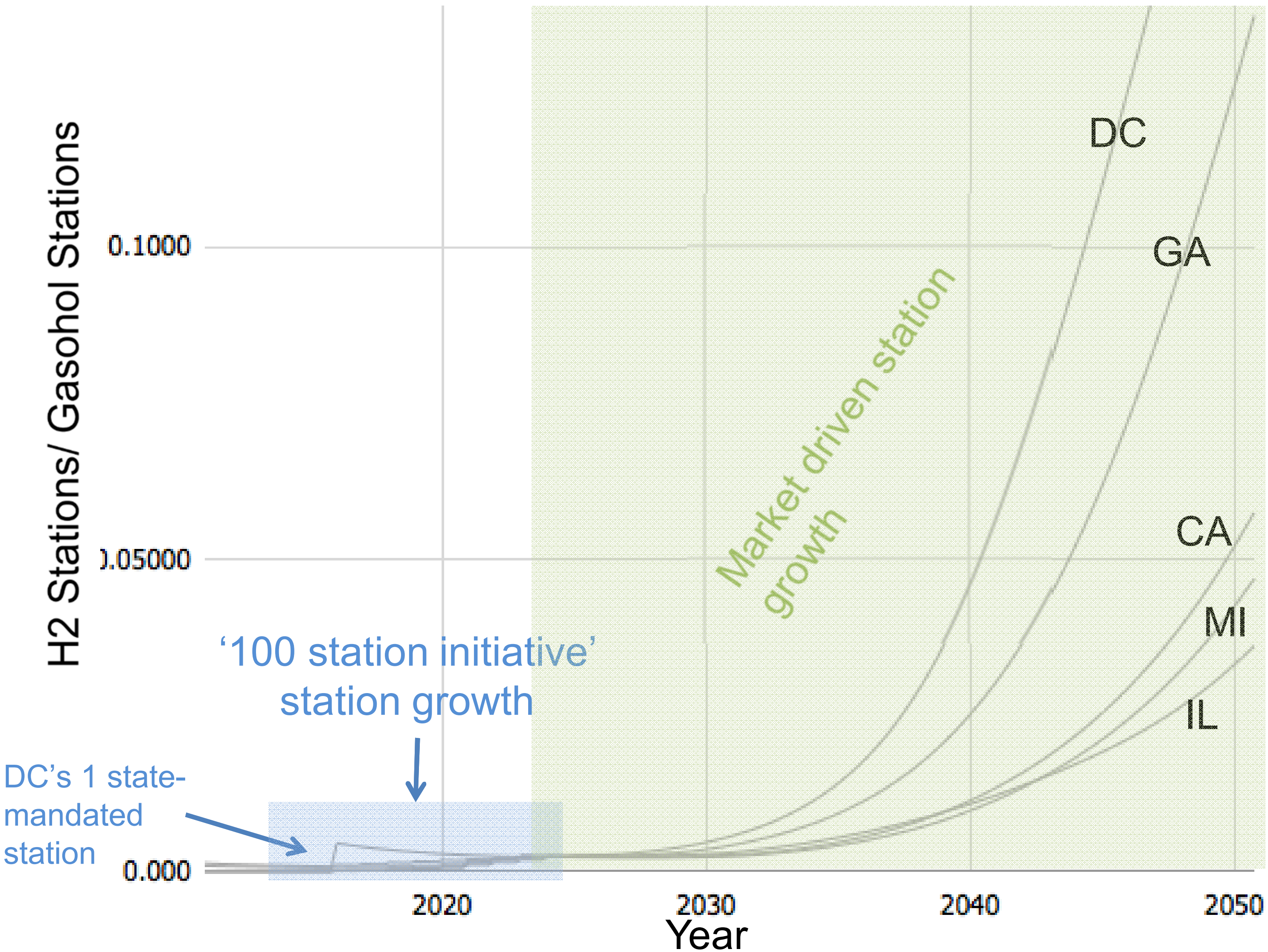


Most refueling stations rely on industrial H2 until the early 2030s. When vehicle demand makes the dedicated production options economical, central coal and distributed SMR become the dominant production pathways.

Case 1: Pump fuel prices



Case 1: Refueling infrastructure



State mandated H2 stations provide a kick-start for station growth, but the majority of growth is market driven, after the initiatives end

Case 3 (Carbon tax): Fleet

Powertrain		ICE	Hybrid	PHEV10	PHEV40	BEV	FCEV	CNG
% of 2050 fleet	No FCEV	34.2	25.8	21.6	6.1	3.2	0.0	9.1
	Base Case	31.8	21.9	17.9	5.3	2.5	14.3	6.4
	Low Cost Electrolysis	30.2	19.2	15.2	4.5	2.1	23.6	5.0
	Carbon Tax	26.5	21.3	17.7	6.5	3.9	17.6	6.3

Pump Fuel		Gasohol	Diesel	E85	NG	H2	Electricity
% of 2050 mileage	No FCEV	63.4	10.9	1.6	11.0	0	13.0
	Base Case	54.0	9.0	1.4	7.5	17.3	10.7
	Low Cost Electrolysis	46.9	7.6	1.3	5.7	29.6	8.9
	Carbon Tax	42.9	7.1	7.3	7.6	21.4	13.4

Carbon tax has a small positive impact on FCEV market share over the base case.
It also positively affects BEV and PHEV adoption, and lowers overall gasohol use.

Reviewer Only Slides

Modeling Approach: Model inputs are taken from published sources when possible, but many are parameterized

Vehicle model

- Consumers do not change vehicle class (size)
- VMT varies by model segmentation, but does not change over time
- LDV stock growth rate is the same as population growth rate (per capita vehicles is constant)
- Consumers have baseline 3 year required payback period with no discounting
- Vehicle efficiency, cost, and battery capacity taken from ANL *Autonomie* 2011 model analysis
- CAFE requirements are satisfied
- Consumer choice model is nested, multinomial logit type (like MA3T)
    - Sale shares depend on amortized consumer *utility cost* = vehicle purchase price – subsidies + fuel operating costs + penalties (range and fuel availability)
- Bi-fuel vehicles (E85 FFVs, diesel vehicles, and CNG bi-fuel vehicle) dynamically choose fuel use rate breakdown using:

(Probability of visiting a station with CNG) * (Willing-to-pay price premium)

Changes as new pumps are added in response to vehicle sales

Responds to market conditions (price sensitivity is parameterized)

Hydrogen production pathway choices necessitates that H2 fuel-production has its own sub-model, distinct from the other fuels.

Available gaseous hydrogen production pathways in the ParaChoice model

- Dedicated distributed production
  - From natural gas with SMR (Dist. SMR)
  - By electrolysis using marginal grid electricity (Dist. Elec.)
- Dedicated central production, gaseous H2 transferred to station by tube truck
  - From natural gas with SMR (Cent. SMR)
  - From coal (Cent. Coal)
  - By electrolysis via renewable energy (Cent. Elec)
  - From natural gas with SMR + sequestration (Cent. SMR Seq.)
  - From coal + sequestration (Cent. Coal + Seq)
- Industrial H2 (Cent. SMR) made available to vehicles at a price markup

Q: What will determine which pathways get used?

- Cost of fuel by pathway
  - New production capacity will optimize for lowest H2 pump-fuel price
- Scale of demand
  - At low demand, dedicated central production is not economically viable
  - At even lower demand, industrial prices may be economically favorable to scaled distributed production
- Renewable fuel mandates

H2 fuel production logic added to the ParaChoice model, and data sources

Init:

- Number of H2 stations is taken from AFDC (~50 nationally, ~20 in CA)
- No pre-existing dedicated H2 production capacity
- H2 prices are assumed to be industrial prices at lowest volume pricing, obtained from Hydrogen and Fuel Cells US Market Report, 2010.

Loop:

- Fleet sets new H2 demand
- By state, if H2 demand > existing capacity: choose between
  - Industrial H2- chosen at very low demand if no dedicated capacity exists
  - Dedicated distributed production
    - Full station capacity is 1,500kg/day (H2A)
    - Prices are scaled up when usage < capacity
  - Dedicated central production
    - Full station capacity is 50,000kg/day (H2A)
    - Only an option if rate of demand increase is at least 12,500 kg/day/year (compliant with H2A assumption of 50,000kg/day plant capacity, 40 year lifespan, and 90% production capacity)
- Retire old production capacity (40 years for central, 20 years for distributed, H2A)
- New H2 prices are supplied to vehicle sub-model to compute new FCEV sales
- Refueling stations are updated based on new FCEV market share

Other model inputs are taken from published sources when possible

Energy sources

- Oil: Global price from EIA Annual Energy Outlook (2014)
- Coal: National price from EIA Annual Energy Outlook (2014)
- NG: Regional price from EIA Annual Energy Outlook (2014)
  - Also use differential prices for industrial, power, and residential uses
- Biomass: State supply curves from ORNL's Billion Ton Study
  - Price corrected to match current feedstock markets

Fuel conversion and distribution

- Conversion costs and GHG emissions derived from ANL GREET model (latest version)
- RFS grain mandate is satisfied first, then cellulosic (but not enforced)
  - Gasohol blendstock allowed to rise from E10 to E15
- Ethanol can be transported from one region to another for cost or supply balance
- Electricity grid
  - State-based electricity mix, allowed to evolve according to population growth and energy costs
  - Intermittent and "always-on" sources assumed to supply base load first
  - EVs assumed to be supplied by marginal mix

Vehicle efficiency and price projections

- *Autonomie* 2011

Details, knobs, and switches

- All pathway H2 prices are individually tunable
  - Multipliers for 2015 and 2050 ‘fixed’ prices (not feedstock or electricity)
  - Price evolves by yearly percent changes, reflecting technology improvements
  - H2 prices reflect both production pathways and age of existing production plants
- Industrial price markup is tunable
  - Industrial H2 prices are expressed as a markup over the price of H2 produced in a Cent. SMR plant dedicated to vehicle H2 production. Nominal industrial H2 prices are taken from the Hydrogen and Fuel Cells US Market Report, 2010 (MR2010).
  - Markup varies with scale of demand, reflecting MR2010 values
- Option for initial H2 production capacity (default = No)
  - Initial capacity is assumed to be Dist. SMR at 1500kg/day production
  - H2 prices start at full scale distributed production rates

Details, knobs, and switches

- Option for state sponsored station growth akin to CA's 100 station initiative (default = Yes)
  - Number of mandated stations per state is 100x the ratio of 2015 petrol stations in the state as compared to CA
  - Growth follows national CNG station growth trends
  - Implemented to get around a bootstrapping issue for vehicle/station growth in states with 0 H2 stations at the start of FCEV market introduction in 2015. Turning the option off decreases the 2050 FCEV fleet fraction by less than 5%.
- Optional renewable mandate for production pathway
  - Can choose goal fraction of H2 produced by renewable pathways and goal year
  - Mandated renewable fraction updates yearly, and increases linearly until goal year
  - Mandate will force any new capacity built to comply (i.e. if additional non-renewable capacity will drive the total amount of H2 produced out of compliance, only renewable pathways will be allowed to be constructed.)

FCEV and infrastructure assumptions

- Future H2FC performance and cost projections from *Autonomie* 2011 report
  - FC cost is parameterized
- New H2FC vehicle models are made available to consumers using a proscribed growth curve (**not** a dynamic response to sales)
- No home refueling for FCEVs. H2 is only available at public refueling stations
- New H2 refueling stations are added proportional to new H2FCs purchased
  - This growth rate is parametrically variable
  - FCEVs (and other AEVs) are subject to an infrastructure penalty based on station scarcity

H2 pricing, production, and emissions assumptions and data sources

- Energy intensity and efficiency factors for the pathways come from the NREL-Sandia *Macro Systems Model*, which itself aggregates other DOE model inputs (e.g. H2A, HDSAM)
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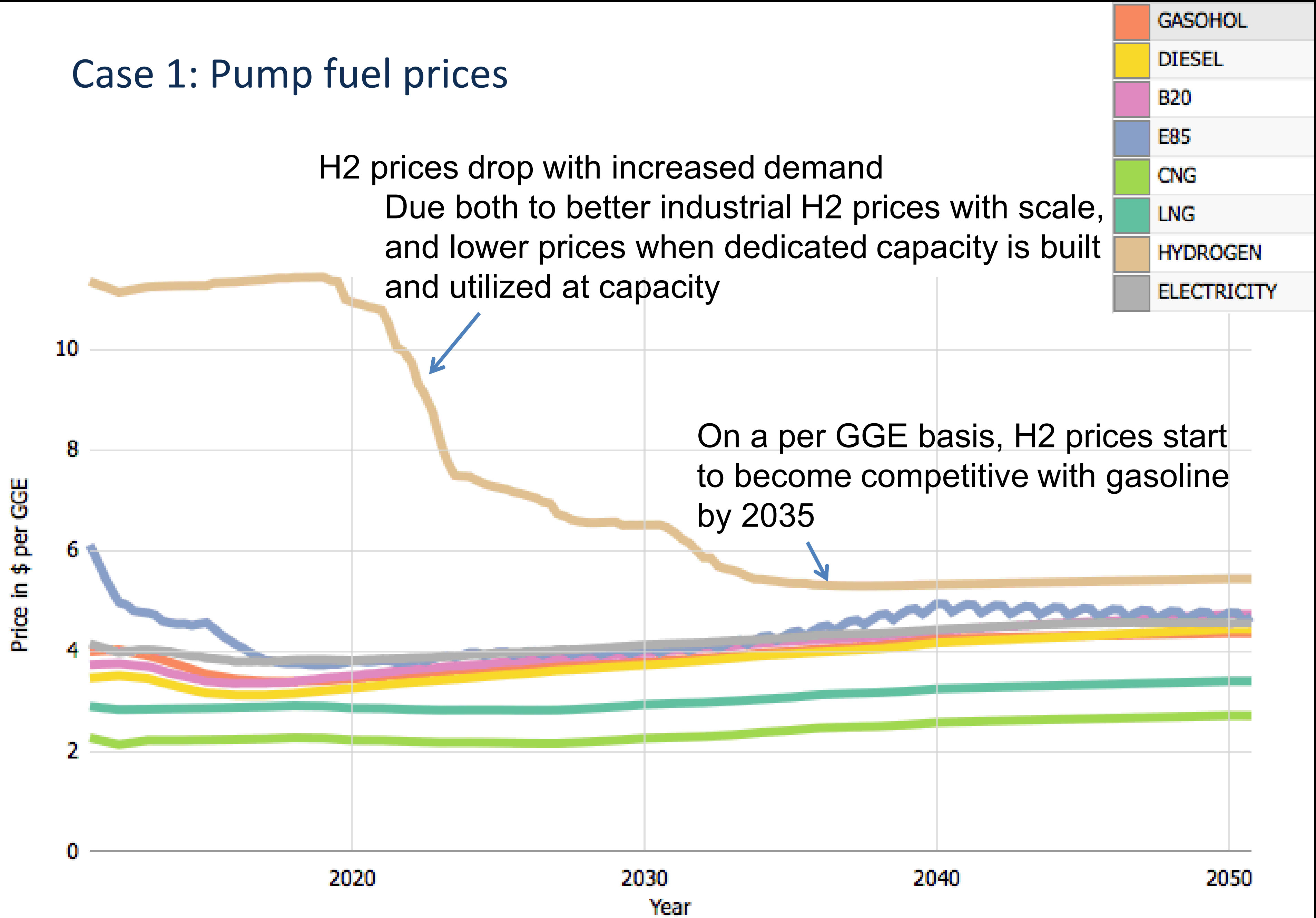
  - Production electricity costs
  - State and federal taxes and fees
  - All other costs (e.g. fixed, O&M) associated with production, transport, and distribution

Pathway	Dist. SMR	Dist. Elec	Cent. Coal	Cent. SMR	Cent Elec.	Coal + Seq	SMR + Seq
Cost at scale (2007$)	4.59	6.61	4.58	5.17	7.51	5.15	5.39

H2 pricing, production, and emissions assumptions and data sources

- H2 prices and emissions evolve in time according to:
  - The evolving mix of production pathways
  - The evolving cost of feedstock fuel (for H2 production and distribution both)
  - The evolving electricity grid mix*
    - H2 fuel costs update with electricity costs, but emissions are NOT updated with the electricity grid (except for production via electrolysis!). Instead, emissions for each production pathway are fixed to the MSM values (2015 US average electricity grid mix). This is consistent with the treatment of other fuels in the model, and is based on the assumption that production electricity contributes very little to the total GHG emissions from fuel production and use.
- Distributed electrolysis is assumed to use the marginal grid mix for each state
  - Same mix as electric vehicle recharging
- No liquefaction step is considered in the pathways
  - Gaseous H2 is transported via tube truck

Case 1: Pump fuel prices



Case 1: Pump fuel prices by mile