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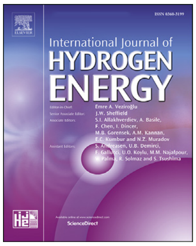

Model to inform the expansion of hydrogen distribution infrastructure

Emily Beagle [a,b], Michael Lewis [b], Braden Pecora [a], Joshua Rhodes [a], Michael Webber [a], Robert Hebner [a,b,*]

[a] Walker Department of Mechanical Engineering, University of Texas at Austin, United States
[b] Center for Electromechanics, University of Texas at Austin, United States

HIGHLIGHTS

- Model developed to support hydrogen infrastructure growth.
- Identified hundreds of solutions to deliver hydrogen to the dispenser at \$4/kg.
- Policies, tax credits, and offsets produce different viable solutions.
- Today, local production is generally less costly than hydrogen distribution.

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ABSTRACT

A growing hydrogen economy requires new hydrogen distribution infrastructure to link geographically distributed hubs of supply and demand. The Hydrogen Optimization with Deployment of Infrastructure (HOwDI) Model helps meet this requirement. The model is a spatially resolved optimization framework that determines location-specific hydrogen production and distribution infrastructure to cost-optimally meet a specified location-based demand. While these results are useful in understanding hydrogen infrastructure development, there is uncertainty in some costs that the model uses for inputs. Thus, the project team took the modeling effort a step further and developed a Monte Carlo methodology to help manage uncertainties. Seven scenarios were run using existing infrastructure and new demand in Texas exploring different policy and tax approaches. The inclusion of tax credits increased the percentage of runs that could deliver hydrogen at <\$4/kg from 31% to 77% and decreased the average dispensed cost from \$4.35/kg to \$3.55/kg. However, even with tax credits there are still some runs where unabated SMR is deployed to meet new demand as the low-carbon production options are not competitive. Every scenario, except for the zero-carbon scenario (without tax credits), resulted in at least 20% of the runs meeting the \$4/kg dispensed fuel cost target. This indicates that multiple pathways exist to deliver \$4/kg hydrogen.

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* *Corresponding author*. Walker Department of Mechanical Engineering, University of Texas at Austin, United States.
E-mail address: r.hebner@cem.utexas.edu (R. Hebner).

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Introduction

Growth of the hydrogen economy requires matching supply and demand, not just at a macro level but also geographically [1]. In an analogous situation, the appropriate distribution of charging stations for battery powered vehicles spawned the development of about fifty different computer-based models to support informed decisions [2]. And, in contrast to the hydrogen infrastructure, underlying electricity infrastructure is near ubiquitous.

The project team developed the Hydrogen Optimization with Deployment of Infrastructure (HOwDI) Model to inform hydrogen supply chain infrastructure development and guide hydrogen investments. This is a spatially resolved optimization framework that determines location-specific hydrogen production and distribution infrastructure to cost-optimally meet a specified location-based demand. This model explores options for hydrogen supply chain infrastructure. This information can help guide the phasing of hydrogen projects. The model runs as a single simulation or in a Monte Carlo framework to better reflect price uncertainties and capture the impacts of future price declines on delivered hydrogen price and infrastructure design.

With the global investment in hydrogen technology, the cost and readiness levels of hydrogen technologies are changing at an unprecedented rate [3]. Current hydrogen cost is about $1/kg at natural gas prices of the decade of the 2010s (approximately $3.50/MMBtu), while hydrogen produced with carbon capture at those same natural gas prices may cost $1.50/kg to $2/kg. The cost of hydrogen produced by an electrolyzer operating on low/zero carbon electricity can be $4/kg to $6/kg, dependent on the cost of the electricity [4]. The model is important because it permits an assessment of the implication of the decreasing costs of hydrogen production and distribution technologies.

Since the expansion of hydrogen infrastructure is influenced by both preexisting infrastructure and by the spatial distribution of demand hubs,[1] the model is structured to use geographically specific inputs with a computational approach that is sufficiently generic to be applicable to a wide range of situations. The initial application of this model is in the state of Texas, part of the USA. Texas has long been a domestic and global energy leader. Not only is Texas a leading producer of oil and natural gas, but it is also the leading domestic producer of wind power and a growing producer of solar power and grid-scale energy storage [5]. It is simultaneously a leading national producer and user of hydrogen: producing, distributing, and consuming about 30% of the hydrogen produced annually in the United States or 3% of hydrogen consumed globally [6]. Thus, as it did with natural gas production, Texas is poised to be among the world leaders in its transition to lower carbon energy sources to mitigate climate change. A critical component to this energy transition is the inclusion and scale up of low carbon intensity, or clean, hydrogen, which can play a major role in decarbonizing transportation, industrial feedstocks, and the energy sector. Major oil and gas companies are leading this transition by expanding their portfolios to include clean hydrogen in lockstep with renewable energy companies [7–9]. They provide Texas and the US with an example of how to realize and manage the transition.

Literature review

Extensive work has previously been done investigating hydrogen's use in the transportation sector with a particular focus on hydrogen refueling stations (HRS). Research topics span station location optimization, technoeconomic analysis, and investigation of specific station equipment performance [10]. As hydrogen fuel cell electric vehicles have been deployed in select locations around the world, data and analysis of HRS performance have become available [11]. Genovese et al. [12] used four years of data (2016–2020) from the California State University Los Angeles Hydrogen Research and Fueling Facility to evaluate energy and other key performance metrics of the fueling station in real-world conditions. Over this time period, improvements in station components and increases in hydrogen demand improved overall station energy usage. Gao and Zhang [13] used a system dynamics model with data from California fueling stations to examine the effect of government funding and policy support for decentralized/localized hydrogen production on-site at hydrogen refueling stations. They found that public funding can help establish hydrogen technology adoption in the early stages of market development.

Capacity expansion models are a commonly used tool to model macro energy systems and infrastructure interaction and development. These are most often used to model the electricity system, though several are being developed that integrate the electric sector with hydrogen infrastructure [14–16]. All capacity expansion models require that resource supply (usually electricity) is greater than or equal to the resource demand. This is a reasonable assumption for the electric sector, as consumers will purchase electricity regardless of the price and the practical functioning of the grid system is that demand must always be met with supply. However, it is difficult to justify this constraint when modeling hydrogen capacity expansion as potential hydrogen demand sectors will only purchase hydrogen if it is economical to do so and other alternative fuels for end use sectors currently exist.

These previous studies have assessed the technical needs and performance of hydrogen refueling stations (HRS) as they operate independently or with localized and decentralized hydrogen production. Other systems level modeling of HRS have been used to determine the optimal location for such facilities within city boundaries or regions of other sizes. Capacity expansion models have been expanded to include hydrogen in integrated energy systems with fixed requirements to meet demand for both commodities.

The novel contributions of this study can be summarized as follows.

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[1] In the HOwDI model context, ‘hub’ refers to a location with a collection of nodes of production, consumption, and distribution. The US Department of Energy administers a Regional Clean Hydrogen Hubs program to increase the number of such hubs in the US. The HOwDI model is applicable to new hubs stimulated by that government-led program but is designed for broader application.

- This model specifies the location of demand (and by extension fueling stations) and optimizes for the hydrogen production and distribution infrastructure to supply this demand. This is an important contribution to the literature because as hydrogen is being deployed economy wide and as hydrogen use in the transportation sector and other sectors grows, it is likely that initial projects will focus on where demand is for hydrogen fuel and the supply chain to meet that demand will need to be built.
- Additionally, since cost is one of the largest barriers to widespread hydrogen adoption, the HOwDI model's ability to evaluate the delivered price of hydrogen at set demand locations and identify critical technologies for reducing the cost, is an important contribution to the scientific literature.
- The model is constructed such that the specified hydrogen demand does not have to be met if hydrogen cannot be delivered for less than a willingness-to-pay parameter. This better simulates the realities of the emerging hydrogen economy and distinguishes HOwDI from most other models that force demand to be met regardless of cost or will not solve without all demand being met.
- The Monte Carlo formulation of the model is used to identify technology improvements and cost declines that are most critical to realizing a competitive price of delivered hydrogen in new applications. These insights can be used to better direct research funding and efforts.
- The model scenarios presented demonstrate the importance of the new clean hydrogen production tax credits in the United States on making the cost of clean hydrogen competitive and allow for investigation of the impacts of other policies on system level hydrogen deployment and costs.

Hydrogen infrastructure modeling

The Hydrogen Optimization with Distribution of Infrastructure (HOwDI) model [17] incorporates hydrogen infrastructure across the supply chain including production, conversion, distribution, and end-use. The model is a python based mixed-integer linear program (MILP) that maximizes system-level profit balanced with the costs of building and operating the required hydrogen infrastructure. The model objective is defined as:

$$\max\left(Utility_{H_2} - Costs_{infrastructure}\right)$$

where:

$$Utility_{H_2} = (sector\ willingness\ to\ pay\ price)*(hydrogen\ consumed)$$

Hydrogen production methods in the model include steam methane reforming (SMR) with various carbon capture rates and electrolysis with various levels of assumed renewable electricity input. The model includes conversion processes between liquid and gaseous hydrogen as needed throughout the system. The three mature approaches to hydrogen distribution are included in the model: compressed gas pipelines, liquid trucking, and compressed gas cylinder trucking. Metal hydrides and ammonia for reversible hydrogen storage can be added to the model as commercial applicability is better quantified.

Necessary physical constraints are built into the model, including conservation of mass and flow constraints for hydrogen moving through nodes and distribution systems. The possible hydrogen producers (SMR and electrolysis) have minimum and maximum production capacities that represent real world size considerations. These size constraints were informed by discussions with project partners during the model design process.

While the model can capture hydrogen consumption in a variety of sectors, the initial model application explored hydrogen infrastructure needs as fuel for heavy-duty transportation so the end-use considered includes demand and associated costs for building hydrogen fueling stations in locations with user-defined hydrogen demand.

The model includes the geography of the existing Texas hydrogen system, including the hydrogen production and consumption at various hydrogen hubs around the state, as well as the hydrogen distribution system. Fig. 1 shows the network model logic and area of consideration. At each hub, the model can build production, conversion, distribution, and/or consumption infrastructure to provide hydrogen for consumers.

Fig. 2 represents one model run, i.e., the optimal deployment of infrastructure given a set of assumptions about infrastructure, energy, and feedstock costs as well as assumptions for any policy-driven tax credits. As shown, the results include spatially resolved hydrogen production and consumption and associated distribution infrastructure by type and volume across the hubs considered in the state of Texas. While these results are useful in understanding how hydrogen infrastructure might develop, there is a high level of uncertainty associated with some of the costs that the model uses for inputs. Thus, the project team took the modeling effort a step further and developed a Monte Carlo methodology to address the uncertainty in the inputs.

Monte Carlo model development

Because the model's linear formulation yields a short solve-time, the modeling team parameterized the domain space and ran the model using a Monte Carlo approach to solve using random combinations of input prices and conditions. In each run, a variable is randomly and independently chosen from each input distribution as an input and each of the HOwDI runs contributes to the development of a distribution of outputs. The set of input and output distributions helps identify which input conditions lead to the desired outputs. This model structure permits the exploration of various pathways and scenarios to determine which model inputs are most important to achieving broader hydrogen deployment goals, delivered price targets, namely $4/kg at the “fuel pump”. Fig. 3 summarizes the Monte Carlo simulation method with a subset of input variables and an example output distribution.

Input parameters

The model includes cost inputs, including production, distribution, conversion, and consumption. A subset of the cost

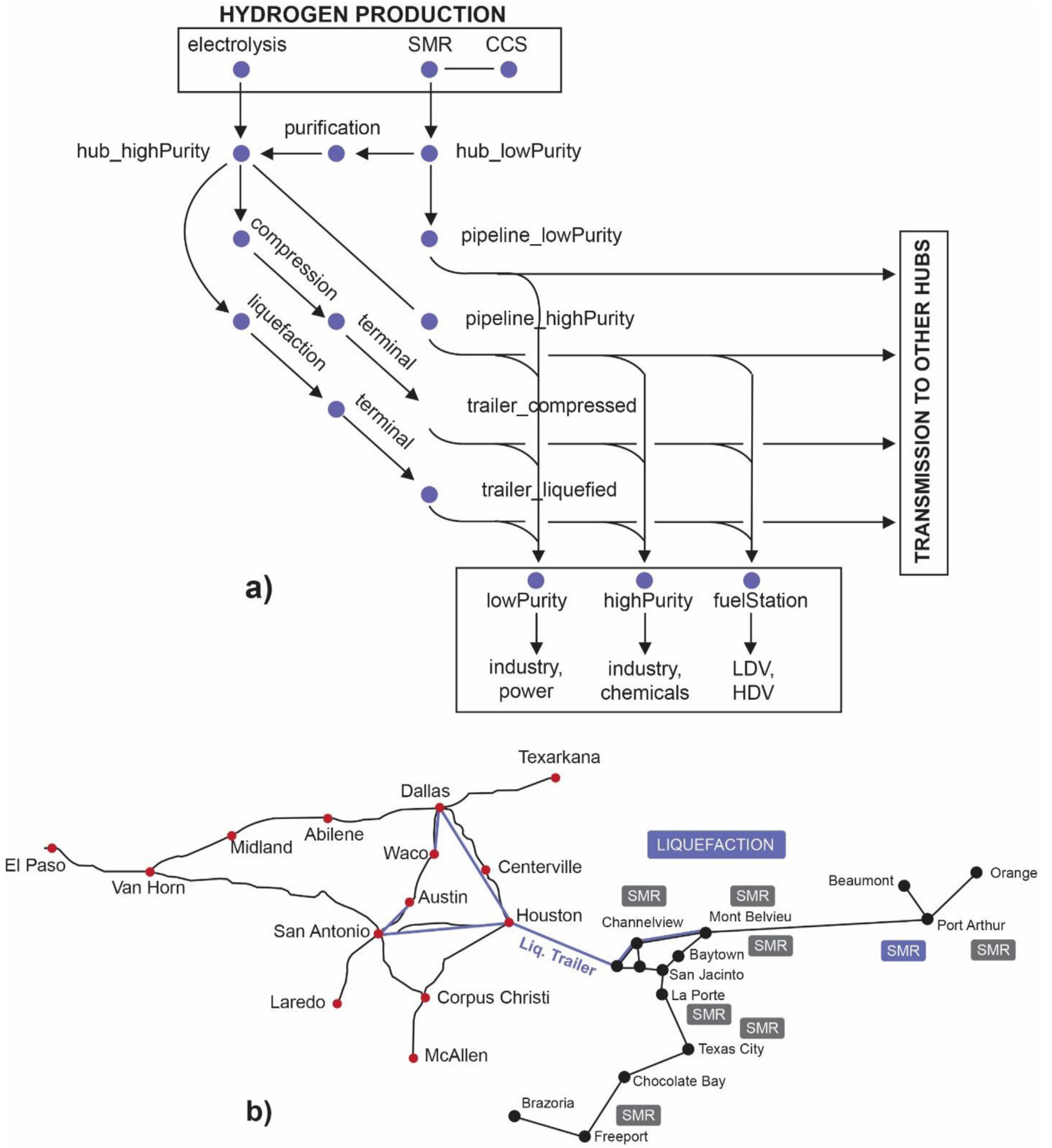

Fig. 1 – Schematic representation of the Hydrogen Optimization with Deployment of Infrastructure model demonstrating the a) network system of the model design and b) the geographical span of Texas and associated hubs included for model runs in this report. Hubs denoted with SMR or liquefaction represent locations of existing hydrogen infrastructure of that type which is included in the model configuration.

inputs was varied from run-to-run during the Monte Carlo simulation scenarios. The varied cost parameters were selected because they either are inputs that are expected to see significant cost declines in the future (such as electrolyzer Capex) or there is significant uncertainty in current costs (such as fuel dispenser). Each parameter was assumed to vary based on a Gaussian distribution. The Monte Carlo input parameters, including the mean and standard deviation of the assumed distribution are in Table 1. Linked variables were also linked for the Monte Carlo variation. For example, the

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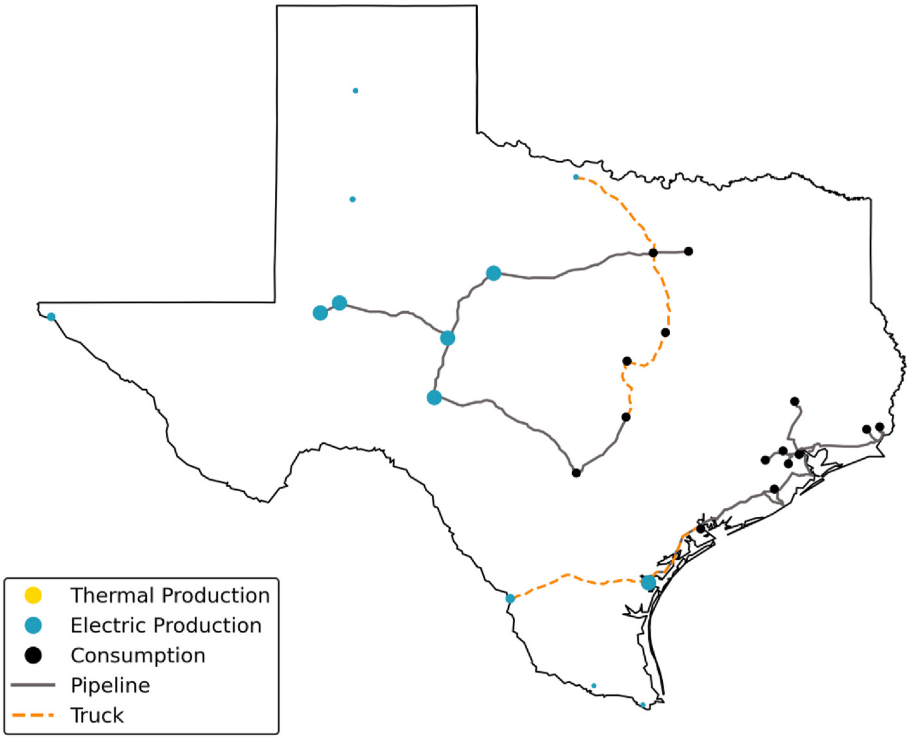

Fig. 2 – Sample outputs of model – spatially resolved hydrogen production and distribution infrastructure.

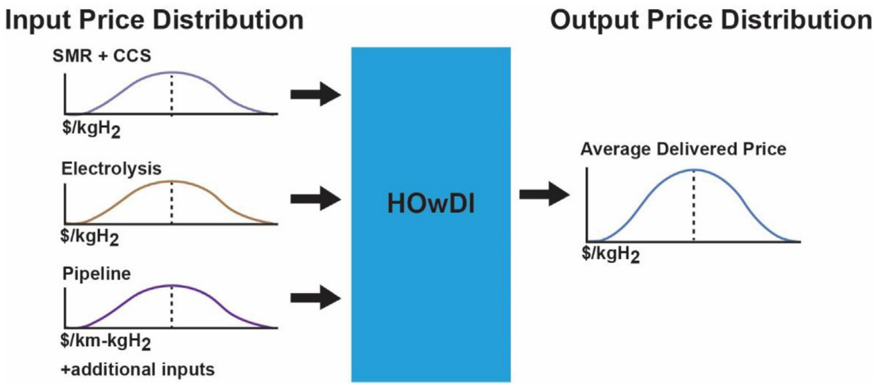

Fig. 3 – Demonstrative figure of the Monte Carlo simulation method showing sample distributions of model input variables and the resulting distribution for a sample output variable of interest.

Table 1 – Input parameters and respective value for Monte Carlo simulations.

Parameter	Mean	Standard Deviation	Unit	Notes
Pipeline - Capex	3,000,000	±25%	$/km	
Compressed Hydrogen Truck - Capex	600,000	±20%	$/truck	
Liquified Hydrogen Truck - Capex	1,000,000	±20%	$/truck	
Liquefaction Facility - Capex	2,500,000	±20%	$/ton/day	
Fuel Station Capex (gas)	15,000,000	±25%	$/ton/day	
Fuel Station Capex (liquid)	10,000,000	±25%	$/ton/day	
Fuel Station Capex (pipeline)	5,000,000	±25%	$/ton/day	
Electrolyzer - Capex	1000	±25%	$/kW	
Steam Methane Reformer - Capex	2,000,000–4,300,000	±25%	$/ton/day	Dependent on capture rate
Electricity Price	0.039–0.055	±25%	$/kWh	Spatially dependent
Natural Gas Price	4.004–4.657	±25%	$/mmbtu	Spatially dependent

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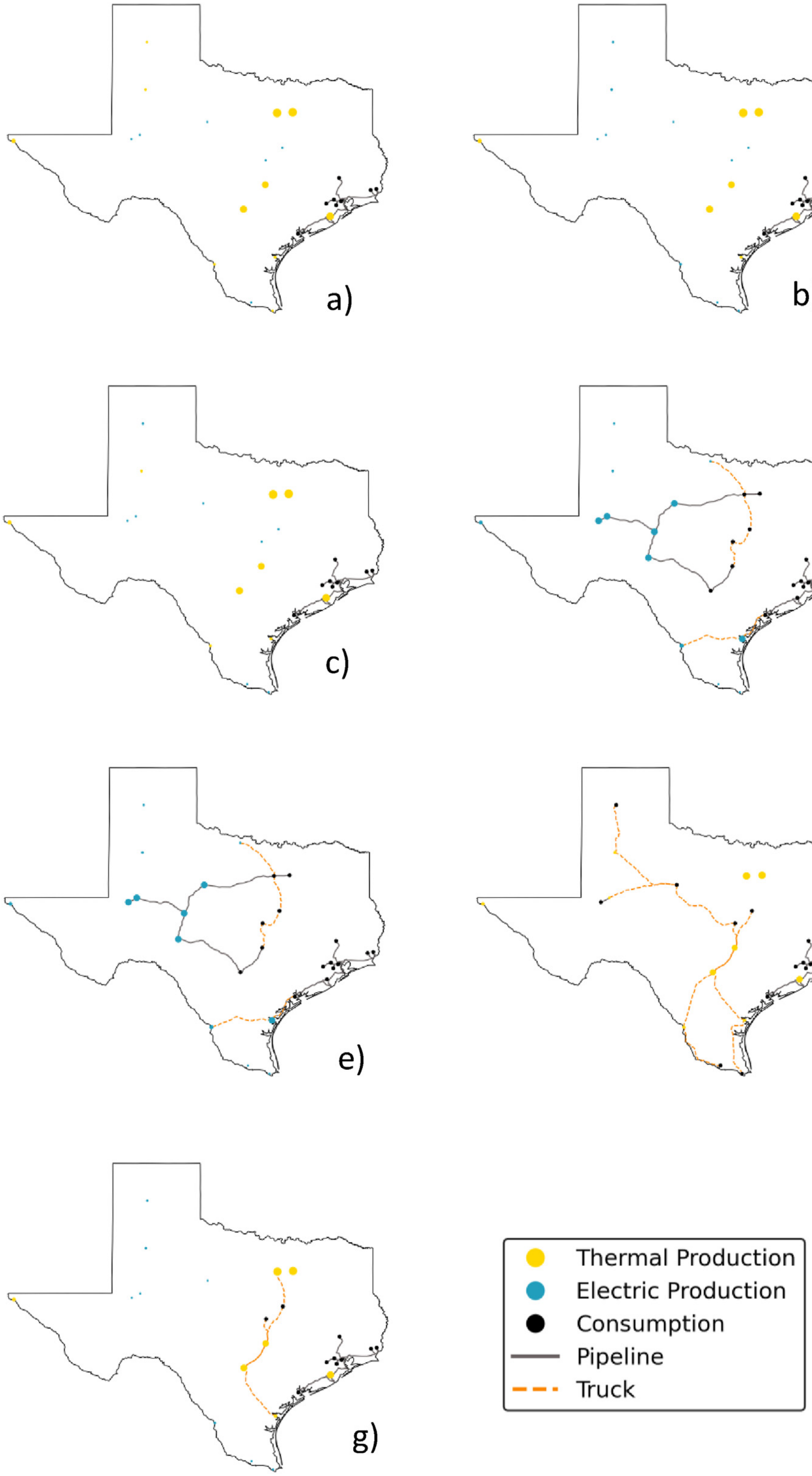

Fig. 4 — **Output maps from individual HOwDI runs for a) baseline, b) low carbon, c) tax credits, d) zero carbon, e) zero carbon tax credits, f) zero carbon with DAC offsets, and g) zero carbon with DAC offsets and tax credits scenarios.**

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Table 2 – Table showing summary statistics of the various Monte Carlo scenarios in this analysis.

Scenario Name	Tax Credits	% runs ≤ \$4/kg	Average Dispensed Cost (\$/kg)	Majority Deployed Technology	Most Correlated Variables
Baseline	No	71%	\$3.69	SMR	Fuel Station[a] & SMR CAPEX, NG price
Low Carbon	No	31%	\$4.35	SMR with CCS	Fuel Station[a] & SMR CAPEX, NG price
Tax Credits	Yes	77%	\$3.55	SMR/SMR with CCS	Fuel Station[a] & SMR CAPEX, NG price
Zero Carbon	No	0%	\$8.32	Electrolysis + RE	N/A
Zero Carbon + tax credits	Yes	33%	\$4.48	Electrolysis + RE	Fuel Station[a] & Electrolysis CAPEX, electricity price
Zero Carbon with DAC offsets	No	20%	\$4.59	SMR with CCS + DAC	Fuel Station[a] & SMR CAPEX
Zero Carbon with DAC offsets + tax credits	Yes	60%	\$3.79	SMR with CCS + DAC	Fuel Station[a], SMR & Electrolysis CAPEX, electricity & natural gas price

[a] Pipeline fed fuel dispenser.

model has inputs for three different types of SMR production facilities: SMR, SMR +60% CCS, and SMR +90% CCS. While each of these has a different base Capex cost, the variation from this base was kept the same for the three technologies in each of the Monte Carlo runs such that if the unabated SMR Capex was 0.8 times its mean for a Monte Carlo run, the SMR +60% CCS and SMR +90% CCS Capex costs were also 0.8 times their mean. Similar linked distributions also apply to electrolyzer capex, natural gas price, and electricity price.

In addition to cost inputs, the model also considers technical specifications of the various hydrogen technologies, such as electrolyzer electrical efficiency, SMR natural gas consumption, and CCS capture rates.

Modeling results

This section provides results from multiple scenarios to highlight applications. The team chose 1000 HOwDI model runs for each Monte Carlo scenario because the results indicated that 1000 HOwDI model runs in each Monte Carlo scenario captured a similar range of inputs and outputs.

The scenarios highlight the influence of various technologies and policies on the cost of hydrogen dispensed at fueling stations across Texas. The HOwDI scenarios reported are.

- **Baseline**: no policy or carbon constraints (business as usual)
- **Low Carbon**: all new hydrogen production built restricted to low carbon technologies.
- **Tax Credits**: any new hydrogen production allowed with inclusion of hydrogen and carbon capture tax credits for eligible technologies.
- **Zero Carbon**: all new hydrogen production built restricted to zero-carbon technologies (electrolysis powered with renewable energy)
- **Zero Carbon Tax Credits**: all new hydrogen production built restricted to zero-carbon technologies (electrolysis powered with renewable energy) with inclusion of hydrogen and carbon capture tax credits.
- **Zero Carbon with Direct Air Capture (DAC) offsets**: all new hydrogen production built restricted to zero-carbon technologies with inclusion of option to 'offset' remaining emissions with direct air capture to meet zero-carbon threshold.
- **Zero Carbon with DAC offsets and tax credits**: all new hydrogen production built restricted to zero-carbon technologies with inclusion of option to 'offset' remaining emissions with direct air capture to meet zero-carbon threshold and with inclusion of hydrogen and carbon capture tax credits.

Fig. 4 shows the geospatial results for individual HOwDI runs for the seven scenarios considered. As a collection, these maps demonstrate the difference in the optimized hydrogen infrastructure system driven by policies and technology restrictions. In the baseline, low carbon, and tax credits case, no new distribution infrastructure (pipeline or truck) was built to supply hydrogen. Rather hydrogen production was built at the hub of demand. When the restriction to build with zero carbon production was introduced, distribution infrastructure is built to move hydrogen from areas of production to areas of demand. Even in the baseline scenario, with no technology restrictions or tax credits, small scale electric production is built to meet small demand in isolated hubs.

While illustrative of the model capabilities and offering some insights into hydrogen development in Texas, the results of the individual runs shown in Fig. 4 do not capture the impact of various price uncertainties on the final model results. The use of the HOwDI model in its Monte Carlo formulation addresses those uncertainties and provides additional insights into the preferred technology pathways and delivered hydrogen costs for a wide variety of input conditions. Table 2 summarizes the Monte Carlo results for the scenarios considered.

Every scenario, except for the zero-carbon without tax credits scenario, resulted in at least 20% of the runs being able to meet the \$4/kg dispensed fuel cost target. That means that at least 200 of the 1000 runs in each scenario were able to meet the cost target. This indicates that multiple pathways exist to deliver \$4/kg hydrogen at the pump. In general, tax credits lower the expected delivered cost of hydrogen, but are not always enough to incentivize the deployment of the technologies that they target, for example, the model often chose to deploy SMR without CCS even when tax credits were available for SMR with CCS or electrolysis.

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No scenario deployed a majority of electrolysis units to meet new demand unless the scenario was restricted from deploying new SMR units via carbon constraints. Even at a levelized \$200/tonne of CO_2 direct air capture abatement costs, the model still showed a strong preference for deploying coupled SMR + CCS with DAC to achieve net zero overall emissions over deploying renewable energy powered electrolysis. All scenarios that were able to dispense \$4/kg hydrogen saw a strong correlation between the capital costs of fuel stations and the final delivered hydrogen cost. This was most apparent in those applications receiving hydrogen via pipelines instead of trucks. While some runs saw a few truck routes or hubs connected via some short pipelines, the majority preferred to build hydrogen production facilities at the same location as the fueling station to minimize distribution costs.

Conclusion

A model is advantageous as a decision-support tool to find cost effective approaches to supplying hydrogen to emerging demand. The HOwDI model is an important contribution as it highlights multiple approaches to achieving the desired delivery cost, the largest cost drivers in each scenario, and potential effects of policy decisions. The capability is useful because of the multiple infrastructure options available, the emerging technology that is affecting the component costs, and the varying policy structure. The model combines all of these to produce a set of cost-optimal options.

The model found that, across a variety of scenarios and input cost considerations, hydrogen could be delivered across Texas for the target cost of \$4/kg at fueling stations. The Monte Carlo formulation of the model allowed for examination of cost input effects on total delivered price for multiple supply chain components and found that, across the scenarios considered, the fueling station cost was a significant driver of total delivered cost. This helps identify areas where technology improvements and cost declines would be most significant towards making hydrogen competitive. Additionally, the model demonstrated the impact that the new clean hydrogen production tax credit will have on reducing the delivered cost of hydrogen.

As the hydrogen industry grows, the model will also need to grow in complexity. One obvious example is that the model assumes that the other infrastructures, such as the electricity infrastructure, are adequate to support hydrogen growth. While this may be true on the macro level for some time, challenges will arise on the geographically resolved level [18].

A second obvious addition to the current model is to include hydrogen storage. Not only is hydrogen stored in pipelines and tanks, but commercial underground storage of hydrogen is also a mature industry [19]. But suitable underground storage capability only occurs in certain locations. Modeling is required to assess the impact of the cost due to the lack of congruence between the locations' high demand and large-scale storage capability.

Cal State Los Angeles [20] reported that their system had a hydrogen loss from production to dispenser of 2%–35%. As experience permits the more detailed documentation of loss in commercial systems, the HOwDI model can expand to include these rates. This information will provide more precise cost estimates of the different technical alternatives.

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Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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