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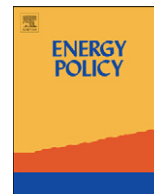
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The role of biomass in California's hydrogen economy

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ABSTRACT

This paper presents the results of a model of hydrogen production from waste biomass in California. We develop a profit-maximizing model of a biomass hydrogen industry from field to vehicle tank. This model is used to estimate the economic potential for hydrogen production from two waste biomass resources in Northern California—wheat straw and rice straw—taking into account the on the ground geographic dimensions of both biomass supply and hydrogen demand. The systems analysis approach allows for explicit consideration of the interactions between feedstock collection, hydrogen production, and hydrogen distribution in finding the optimal system design. This case study approach provides insight into both the real-world potential and the real-world cost of producing hydrogen from waste biomass. Additional context is provided through the estimation of California's total waste biomass hydrogen potential. We find that enough biomass is available from waste sources to provide up to 40% of the current California passenger car fuel demand as hydrogen. Optimized supply chains result in delivered hydrogen costing between \$3/kg and \$5.50/kg with one-tenth of the well-to-wheels greenhouse gas emissions of conventional gasoline-fueled vehicles.

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1. Introduction

Both hydrogen and biomass-based fuels have received significant attention as future transportation fuels in recent years (IEA, 2005; NRC, 2004). The interest in these alternative fuels rests on their potential societal benefits including the possibility for deep reductions in well-to-wheels greenhouse gas emissions, and diversification of primary supply for transportation fuels away from dependence on petroleum. Hydrogen has the added benefit of zero tailpipe emissions.

Hydrogen's environmental benefits vary greatly depending on the primary energy source used to make hydrogen (IEA, 2005; Milliken et al., in press). One of the key questions is whether hydrogen can be produced at low cost with low emissions. Unfortunately, the most environmentally friendly hydrogen pathways tend to be the most expensive. Hydrogen from wind and solar could tap into vast, zero carbon resources, but are significantly more expensive than hydrogen from fossil sources (natural gas and coal), routes that, without carbon sequestration, offer modest or no benefit compared to gasoline hybrid vehicles (Milliken et al., in press; NRC, 2004). Biomass is a potentially interesting source for hydrogen as it could provide most of the environmental benefits of wind or solar hydrogen, at costs closer to those of hydrogen from natural gas or coal.

The near- and long-term outlook for biomass hydrogen is unclear. A recent study by the National Academies found that biomass hydrogen would be much more costly than hydrogen from natural gas or coal, suggesting a minor role, if any, for biomass hydrogen (NRC, 2004). Other studies suggest biomass hydrogen could be more competitive (Hake et al., 2006; Hamelinck and Faaij, 2006; Meyers et al., 2003). There is little consistency among these studies, and none have examined hydrogen in the context of the full biomass energy system. Clearly, biomass hydrogen faces several questions that need to be clarified in order to properly understand its place in the suite of future hydrogen supplies:

- Is there enough biomass to make a significant contribution toward fueling the transportation sector?
- Is biomass hydrogen economically viable? How would it compete with other near- and long-term sources of hydrogen?
- What are the environmental impacts of using biomass for hydrogen production, particularly with respect to carbon emissions?

Answering these questions in general is difficult due to the highly variable, geographically specific, nature of biomass resources. Different biomass resources are available in different regions. In addition, the density of the available feedstock can vary greatly between regions. The geographic variability is especially important due to the low energy density of both biomass and hydrogen, which leads to high transportation costs. It is, therefore,

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crucial to consider the geographic context in making an assessment on the viability of biomass hydrogen.

The entire biomass hydrogen system, including biomass harvesting, biomass storage and transport, biomass conversion to hydrogen, and hydrogen delivery to users (see Fig. 1) must be considered in assessing biomass hydrogen. The costs of the biomass feedstock, hydrogen production and hydrogen delivery depend sensitively on scale and spatial layout (location and density of biomass resources and hydrogen users). Moreover, these costs are interdependent. For example, increasing the size of a production facility decreases the production costs through economies of scale but increases feedstock costs through increased transportation distances. Previous biomass hydrogen studies have not adequately considered the system as a whole, which has led to widely divergent delivered cost estimates for biomass hydrogen among different studies.

In this paper, we begin to tackle the questions stated above using a detailed case study of the hydrogen production potential from waste biomass in California. California is of particular interest for hydrogen research because of a wide range of policy measures encouraging low-carbon fuels in general (California Governor's Office, 2007; California State Assembly, 2006; Farrell and Sperling, 2007) and hydrogen in particular (Cal/EPA, 2005). Waste biomass resources are promising in California, especially in the near term. A recent assessment by the California Biomass Collaborative shows that biomass waste streams could be a significant resource: 24.3 million dry tons (1 ton = 1 Mg = 1000 kg = 1.102 short tons) of biomass were available in 2005 (CEC, 2004). Costs for waste biomass can be low or even negative. In addition, waste biomass resources do not pose a food versus fuel dilemma for the use of agricultural land. By contrast, the energy crops undergoing most research, switchgrass and short-rotation tree crops, are unlikely to play a major role in California (De La Torre Ugarte et al., 2003).

We explore the premise that in California, significant contributions could be made using waste biomass to fuel vehicles with hydrogen. To study biomass hydrogen systems, we have developed a mathematical model, which considers the biomass resources, hydrogen demands and prices to find the quantity of hydrogen from biomass that is likely to be made available. In the process, optimal biomass supply chains are found. Two important biomass waste feedstocks—rice straw and wheat straw—are used to demonstrate the model and give representative results for biomass hydrogen production supplies and costs.

2. Potential hydrogen production from waste biomass supply in California

Hydrogen production from California's diverse waste biomass resource base can be accomplished with two technologies,

gasification and biogas reforming. Gasification produces hydrogen from dry biomass feedstocks (i.e. straws, stovers, and woody biomass). Most estimates report gasification conversion efficiency between 51% and 65% (Hamelinck and Faaij, 2002; Katofsky, 1993; Larson et al., 2005; Lau et al., 2003; Simbeck and Chang, 2002; Spath et al., 2003, 2005). To be conservative we assume 55% conversion efficiency. Biogas, a methane-rich gas, can be produced from the wet biomass feedstocks (manures, urban green waste, and food processing wastes) through anaerobic digestion. Biogas, landfill gas, and wastewater biogas are all methane-rich gases that can be converted to hydrogen through steam methane reformation. Current practice steam methane reformers achieve 70% efficiency (NRC, 2004). Biogas reformers may be less efficient; therefore, we assume 65% conversion efficiency for biogas to hydrogen.

We estimate that waste biomass resources in California could provide 335 petaj (1 petajoule = 1 PJ = 10¹⁵ J) of hydrogen energy for transportation fuel. As seen in Fig. 2, the biomass in municipal solid waste represents the single largest resource available for exploitation. Waste products from various forestry operations, including forest and chaparral thinning operations for fire prevention, are the four next largest resources. Other important resources are the residues from orchards and field crops and landfill gas.

On an energy basis, the total biomass hydrogen production potential represents energy equivalent to 16% of the gasoline consumed in California in 2004 (Kavalec and Stamets, 2003). To assess biomass hydrogen's potential, the greater efficiency of

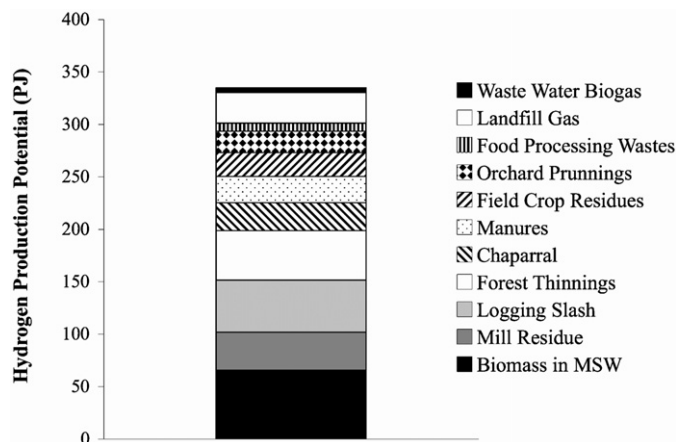


Fig. 2. Total potential hydrogen energy available from waste biomass resources in California. Biomass resource data is taken from California Energy Commission (2004). (1 PJ = 10¹⁵ J = approximately 7 million kg of hydrogen).

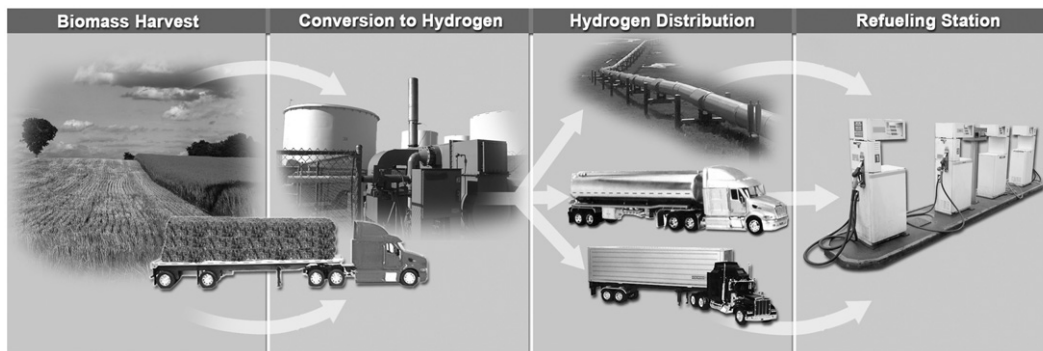


Fig. 1. Simplified picture of hydrogen production from biomass.

a fuel cell vehicle should be taken into account when comparing hydrogen and gasoline. A hydrogen fuel cell vehicle is expected to achieve fuel economies 2.5 times that of conventional gasoline internal combustion engine powered vehicle with the same level of performance (NRC, 2004; Schafer et al., 2006).

As a result, we estimate that 10.1 million vehicles could be fueled by California's biomass hydrogen potential. This assumes hydrogen fuel cell vehicles are driven 19,300 km/year with a fuel economy of 51.5 miles per gasoline gallon equivalent (4.61/100 km), compared with the current fleet fuel economy of 20.6 miles/gallon (Kavalec and Stamets, 2003). For reference, there are currently over 25 million light-duty vehicles in California. In terms of kilometers driven, biomass hydrogen could power vehicles for roughly 40% of current vehicle kilometers traveled by light-duty vehicles. While it is not likely that all the technically available biomass will be economically viable for hydrogen production, this analysis demonstrates that significant contributions to fuel supply are possible from biomass hydrogen.

3. Cost of producing hydrogen via biomass gasification

The supply chain for hydrogen production from biomass has three major stages: biomass feedstock gathering, hydrogen production, and hydrogen distribution (see Fig. 1). This section describes the current state of knowledge for the second stage, hydrogen production. The following section covers hydrogen distribution.

3.1. Hydrogen production

Biomass gasification is the most likely near-term method to produce hydrogen from biomass (Hamelinck and Faaij, 2002; NRC, 2004; Simbeck and Chang, 2002). Gasification is a thermochemical process where the organic compounds of biomass are broken down at high temperature in an oxygen-starved environment. The resulting synthesis gas (or syngas) is primarily hydrogen and carbon monoxide. Fuel cell grade hydrogen is derived by further processing the syngas, and separating pure hydrogen, while emitting carbon dioxide. Electricity can be co-produced with hydrogen. Hydrogen production from biomass gasification exhibits an economy of scale in that larger facilities have lower costs per unit of capacity (Hamelinck and Faaij, 2002). However, large gasification facilities require a large biomass resource which in turn requires the collection of biomass from a large region, increasing the feedstock delivery costs (Cameron et al., 2007; Jenkins, 1997; Kumar et al., 2003).

The production cost of biomass hydrogen varies widely in the published literature and is a source of some contention (Hamelinck and Faaij, 2002; Katofsky, 1993; Larson et al., 2005; Lau et al., 2003; NRC, 2004; Simbeck and Chang, 2002; Spath et al., 2003, 2005). Since no commercial-scale biomass hydrogen production facilities exist, decision makers rely on engineering-economic studies based on technology modeling and expert opinion. The comprehensive study of hydrogen from the National Academies estimates the 'current' technology production cost of hydrogen at \$4.63/kg dropping to \$2.21/kg with 'future' technology (NRC, 2004). Another report from researchers at the National Renewable Energy Laboratory projects the current technology production cost of biomass hydrogen at \$1.46/kg dropping to \$1.31/kg with future technology (Spath et al., 2005). A more optimistic view of the future of biomass hydrogen is offered by Hamelinck and Faaij (2002) showing hydrogen production costs as low as \$1.02/kg after analyzing a number of potential future production facility configurations.

There is no single reason for this large discrepancy in projected production costs reported in the literature. A major factor contributing to the variability is the wide range in the assumed efficiencies of the conversion facility. The National Academies (2004) estimated by far the lowest biomass gasification energy conversion efficiency of 39% compared to the next lowest reported efficiency of 51% (Spath et al., 2005) and highest reported efficiency of 67% (Larson et al., 2005). Studies also show that the co-production of electricity along with hydrogen can improve the economics of hydrogen production (Hamelinck and Faaij, 2002; Larson et al., 2005; Spath et al., 2005).

The size of the production facility is an important factor affecting the unit cost of hydrogen production. Recent engineering-economic studies found that biomass gasification demonstrates significant economies of scale in both capital costs and operational costs, not including feedstock (Hamelinck and Faaij, 2002; Larson et al., 2005; Lau et al., 2003; Spath et al., 2003). In other words, as the gasification facility gets larger, capital and operating costs per kilogram of hydrogen decline. Not coincidentally, the highest cost estimate in the literature is also the smallest production facility. The effect of production facility capacity on the levelized or unit cost of hydrogen is evident in the cost estimates shown in Fig. 3.

The final important factor in the cost of biomass hydrogen production is the cost of the biomass feedstock. The cost of feedstock is dependent on a number of factors. The source of the biomass is important: an energy crop is likely to cost more than a waste product at the source, at least in California (CEC, 2004). Independent of the source of biomass, the yield plays an important role with higher yields leading to lower harvest cost and smaller collection areas for the same quantity of biomass. Finally, the distance biomass must travel to the hydrogen production facility factors heavily in the cost of the biomass feedstock due to the high marginal cost of biomass transportation.

Unfortunately, cost improvements gained by increasing the size of the gasification facility lead to higher biomass feedstock cost due to feedstock transport costs. Sizing a gasification facility to produce the lowest-cost hydrogen requires a tradeoff between economies of scale in production and higher feedstock transportation cost. Furthermore, the feedstock transportation cost is dependent of the geographic layout and density of the resource in a specific region, which could lead to different optimal size facilities in different regions.

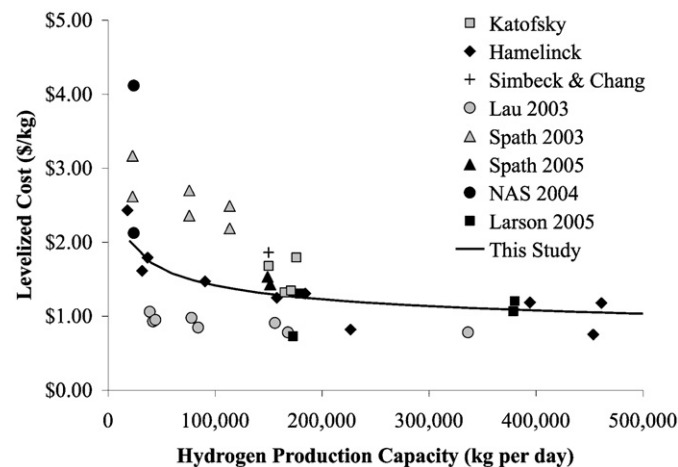


Fig. 3. Projected costs of producing hydrogen through biomass gasification from various sources plotted against the size of the hydrogen production facility. Costs are normalized with \$2/GJ biomass feedstock and 10% internal rate of return on capital.

4. Cost of hydrogen delivery

Biomass gasification is best adapted for centralized production with distribution of hydrogen to refueling stations. We analyze three modes of hydrogen delivery that are used commercially today. Hydrogen can be compressed to high pressures and loaded onto tube trailers for truck delivery. Alternatively, hydrogen can be liquefied at cryogenic temperatures (20K), and delivered in liquid tanker trucks. Finally, hydrogen can be compressed and delivered in a gas pipeline, similar to the natural gas distribution system.

Hydrogen delivery adds significantly to the cost of hydrogen transportation fuel. Delivery system design and cost depend sensitively on the size of the hydrogen demand and the spatial distribution of that demand (Yang and Ogden, 2007). No one mode of delivery is best in all cases. Compressed gas trucks are relatively low cost, but have a low capacity and are best for small, dispersed local demands. Pipelines provide low-cost delivery of large flows of hydrogen and prove to be best for large, dense demands, for example, large numbers of vehicles in a densely populated city. Cryogenic or liquid tanker trucks have low marginal costs of delivery but require the liquefaction of hydrogen, which is expensive in both cost and energy. Liquid trucks are optimal for large demands that are not dense enough to support a pipeline network. In general, large dense demands lead to the lowest delivery costs. Even in the lowest cost delivery scenarios, hydrogen delivery costs can be as high as the cost of hydrogen production (Yang and Ogden, 2007).

In summary, the cost of delivered hydrogen from biomass depends on the size of the production facility, the cost of biomass feedstock, and hydrogen distribution costs. All of these costs depend on the local geography in an optimized system. The complicated nature of hydrogen distribution costs requires that the full system be optimized together: assembling a set of optimized parts will not lead to an optimal system overall.

This work provides a unique contribution to the knowledge of biomass hydrogen production by explicitly considering the complete system to find the optimal hydrogen production supply chain. A further advance is provided by using a sample real-world geographic context for the system.

5. Scenarios of biomass hydrogen in California

The cost of biomass hydrogen is highly dependent on the geography of both the biomass resource and the fuel demand. The tradeoffs between the size of the conversion facility and the cost of feedstock and the location of facility relative to demand and supply will be different for different biomass resources and hydrogen demands. To understand these tradeoffs better, we analyze a number of different possible spatial layouts of biomass supply and hydrogen demand.

Two possible biomass waste feedstocks available in California are examined; rice straw and wheat straw. The two straws represent opposite ends of the spectrum of spatial density for an agricultural waste resource. The rice industry in California is concentrated in a small region where over 25% of the land is devoted to rice production. In contrast, wheat is grown throughout the state (see Fig. 4). The relative density of the rice straw resource is amplified by having 80% higher yields per acre compared to the wheat straw resource. If the full supply of each resource were used to produce hydrogen at 63% thermal efficiency (74.1 kg H₂ per ton rice straw and 77.7 kg H₂ per ton wheat straw), approximately 165 tons of hydrogen per day would be produced. The similarity in potential makes the two resources a good comparison for dense versus dispersed residue resources. These scenarios are meant to be informative about the potential costs of hydrogen from biomass, and allow us to compare a diffuse resource (wheat straw) versus a concentrated resource (rice straw).

The two feedstocks are matched with four hydrogen demand scenarios corresponding to 1%, 10%, 25%, and 50% of the current light-duty vehicle fleet in northern California. The fuel demand is derived from population, with hydrogen demand centers arising in high population density areas. This method of estimating hydrogen demand yields a demand that follows the geographic distribution of population. The 8 pairings of biomass supply and hydrogen demand are analyzed as separate scenarios.

6. Market factors influencing the production of hydrogen from biomass

The market potential of biomass hydrogen will depend not only on the costs of producing and distributing it, but also on the

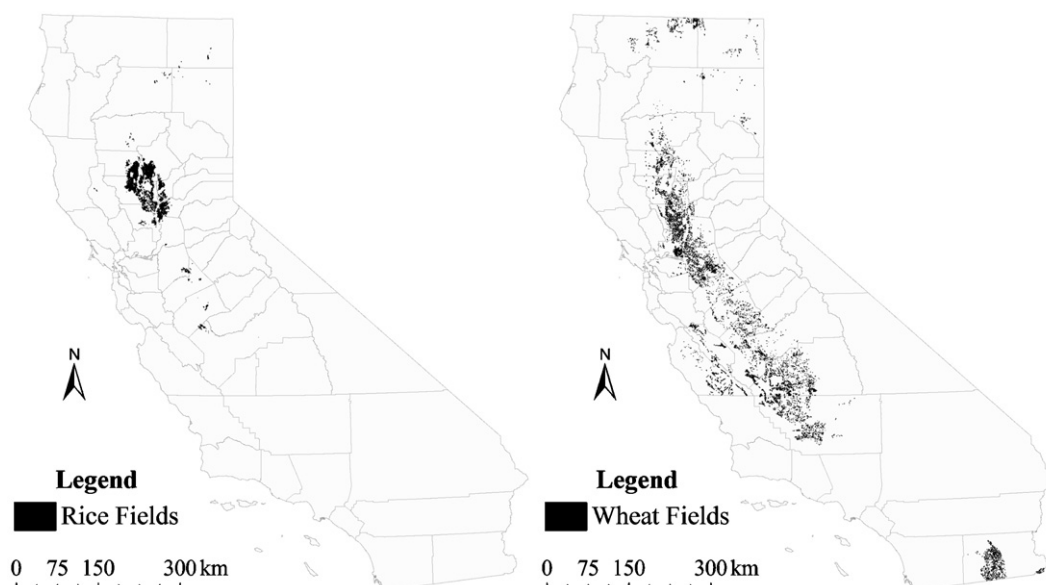


Fig. 4. Location of rice and wheat fields in California; the available biomass resource from the two sources is 772,000 dry metric tons per year for rice straw and 813,000 dry metric tons per year for wheat straw.

future of larger markets for both hydrogen and other biomass products.

Hydrogen can be produced from a wide variety of sources, including natural gas, electricity and coal, as well as biomass (IEA, 2005; NRC, 2004). Competition in the hydrogen market will come from different sources depending on the size of the hydrogen demand. In the early market, the important competitors will be onsite steam methane reformers (SMR) and merchant hydrogen. Onsite SMRs produce hydrogen at the refueling station using natural gas. Merchant hydrogen is delivered from industrial hydrogen producers who mostly serve petroleum refineries and produce hydrogen from natural gas. As the hydrogen market matures, additional centralized sources of fossil hydrogen are expected to come on line, such as hydrogen from coal gasification (NRC, 2004).

Consumers might be willing to pay a premium for renewable hydrogen over fossil hydrogen for two reasons, perceived value for the consumer or government regulation such as a renewable portfolio standard for hydrogen (Cal/EPA, 2005). In this differentiated market for environmentally friendly hydrogen, biomass will compete mostly with onsite electrolysis of water using renewable electricity. The latter source of renewable hydrogen requires significant advances in electrolyzer technology in order to avoid high costs throughout the deployment of hydrogen vehicles limiting its market potential without government intervention (NRC, 2004).

It is important to also understand the opportunity cost of using biomass—or any of these other resources, for that matter—for hydrogen production. Possible competitors for biomass feedstock include liquid biofuels, like ethanol or Fischer-Tropsch diesel, electricity production, animal feed and biomass-based chemicals or plastics. In considering biomass only for transportation fuels, hydrogen promises to be one of the most efficient fuel for converting biomass into vehicle miles based purely on engineering with possible exception of electricity (Hamelinck and Faaij, 2006). The relative economic efficiency of the fuels, however, may not favor hydrogen. If a higher value use of the biomass is available, hydrogen will not be produced from biomass.

These economic factors are included in the analysis presented here by creating a profit-maximizing model for the biomass hydrogen industry. Biomass hydrogen producers are assumed to be price-takers, and the selling price of hydrogen is a model input parameter. The larger market for hydrogen is represented in the model by varying the selling price of hydrogen. In this way, we are able to derive full supply curves for biomass hydrogen—how much would be produced at a series of price points by profit-maximizing producers—rather than assumption-laden single-point estimates.

7. Methods

A profit-maximizing model of the full supply chain was developed to use real-world data on potential biomass supply locations and hydrogen demand. This model describes the optimal behavior of an industry to supply hydrogen transportation fuel from agricultural residues with given hydrogen demand, hydrogen selling price, and feedstock supply. If hydrogen from agricultural residues can be delivered to the refueling stations for less than the given selling price, then it is profitable for the industry to supply that hydrogen and the infrastructure is built to reap that profit. If hydrogen from agricultural residues cannot be delivered for less than the selling price then the hydrogen is supplied by some backstop technology, such as onsite steam methane reforming that is consistent with the given selling price. In addition, when demand for hydrogen exceeds the supply of feedstock, the

difference is made up with hydrogen from the backstop technology.

The model is developed as a mixed integer nonlinear program with the objective to maximize the total biomass hydrogen industry annual profit. Annual revenue from sales of hydrogen and the co-produced electricity are balanced against the annualized cost of capital investments, annual operating costs and the annual cost of biomass feedstock. In maximizing profit, the model chooses where to locate production facilities, the size of each facility, the fields that supply each facility, the demand centers served by each facility, and by which mode the hydrogen is delivered to each demand center. A stylized diagram of the system is given in Fig. 5.

A detailed description of the model equations can be found in the Appendix and in Parker (2007). A basic description of the model is given below by the inputs, outputs and decision variables.

Inputs

- biomass type and supply at each field,
- hydrogen demand for each demand center,
- distances between fields and production sites, production sites and demand centers, and between demand center,
- all costs as functions of component size or flow rate,
- selling price of hydrogen at each demand center.

Decision variables

- size of production facility at each production site (zero is an option),
- size of hydrogen distribution terminal at each production site for each mode of hydrogen distribution,
- quantity of feedstock delivered to each production site from each field,
- quantity of hydrogen delivered to each demand center from each production site by each mode of distribution,
- number of stations in each demand center served by biomass hydrogen specified by mode of hydrogen distribution.

Outputs

- annual profit for biomass hydrogen industry,
- levelized cost (unit cost) of delivered biomass hydrogen,
- optimal values for all decision variables.

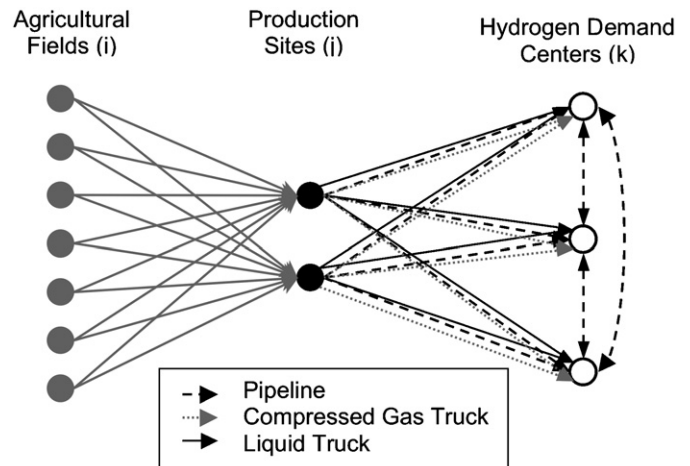


Fig. 5. Diagram of agricultural waste to hydrogen system.

7.1. Choice of modeling framework

We considered two analytic approaches for optimizing biomass hydrogen system; choosing a profit-maximizing framework over a cost minimization one. In many cases, a profit-maximizing model yields the same results as a cost minimization model. However, a profit-maximizing model has several characteristics that make it advantageous over cost minimization for this particular application.

The first advantage of profit maximization is the flexibility it allows to model realistic market factors such as the competition between biomass-based hydrogen and hydrogen from other sources, by using the market price of hydrogen. This differs from cost minimization, which finds the lowest cost biomass hydrogen whether or not it is better than alternative sources. It also captures the tradeoff between the size of a production facility and the cost of feedstock in a realistic manner. Profit maximization allows for optimal facility sizes to be found without the specification of supplies consumed or demands met which are necessary for cost minimization. This provides a good framework for the tradeoff between size and feedstock transportation cost.

The second advantage is in the interpretation of the results. A profit-maximizing approach allows for a direct production of a supply curve for waste biomass-based hydrogen. In contrast, cost minimization produces curves of least cost for given hydrogen produced. The difference is subtle but important. Minimum cost curves do not consider whether it is more profitable to make less lower cost hydrogen or more higher cost hydrogen at a given price. For this reason, minimum cost curves will give the average cost of producing hydrogen at a given quantity while the supply curves will give the marginal cost.

Time variation of demand and supply are not considered here. The results are the optimal decisions for an industry in which the demand and supply are constant for the 15-year lifetime of the production facility. In future work, we will examine the dynamics of increasing demand and building the system over time.

8. Input data for the analysis

8.1. Geographic data

8.1.1. Feedstocks

The location and size of the two biomass resources were determined using the California Department of Water Resources (DWR) land use datasets (2000–2003). These datasets map field-level location data for the state's agricultural industries. The datasets represent a single year's land use. However, the datasets were collected by DWR over a period of 10 years, making the maps an imperfect snapshot of California agriculture. The resource is calculated by applying a per acre yield factor to the fields. Maps of the two resources are found in Fig. 4.

In order to reduce the computational complexity of the model, we reduce the number of distinct fields by spatially clustering the individual fields to a relatively small number of feedstock supply points. This may not be an unrealistic simplification—these supply points can be interpreted as the location of barns or intermediate storage sites where the straw is stored until needed at the production facility.

8.1.2. Hydrogen demand

Hydrogen demand scenarios are developed from population data based on the year 2000 census in the manner described in Ni et al. (2005). Hydrogen vehicle populations were calculated based on 0.7 vehicles per capita and a percentage of total vehicles operating on hydrogen. A fuel demand of 0.6 kg/day per vehicle

was used to derive fuel demand densities. This consumption is equivalent to a 51.5 mile/kg fuel cell vehicle traveling 12,000 miles/year.

Because hydrogen requires a completely new refueling infrastructure, only areas with hydrogen demands large enough to support a station are considered viable locations of hydrogen demand. The areas of high hydrogen demand are aggregated into 'demand centers' (see Fig. 6), which occur in urban areas.

Table 1 summarizes the scenarios. We consider market fractions of 1–50% of vehicles within the demand centers. The market fraction is applied to each demand center and not to the region as a whole. Fig. 6 shows the location of the hydrogen demand centers, considering only northern California demands. Larger demand scenarios increase the size and number of the demand centers.

8.1.3. Potential hydrogen production sites

One of the important model inputs is the set of possible locations for the biomass hydrogen production facilities. Potential hydrogen production sites were selected from the full set of hydrogen demand centers and feedstock supply points by finding the points that would minimize the total cost of delivery of both feedstock and hydrogen. This analysis was performed using hydrogen delivery costs for each of the three modes of delivery (compressed gas truck, liquid truck and pipelines) and for each feedstock. The Richmond and South sites were selected for wheat straw. The Richmond, Sacramento, and North sites were selected for rice straw. The Vacaville and Modesto sites were added to represent compromises between Sacramento and Richmond and Sacramento and South (Fig. 7).

Using a shortest path algorithm within ArcView 3.3, we are able to find the distances between all feedstock supply points and production facility locations, and production facility locations and demand centers over the road network. These distances are used to compute the costs as described below.

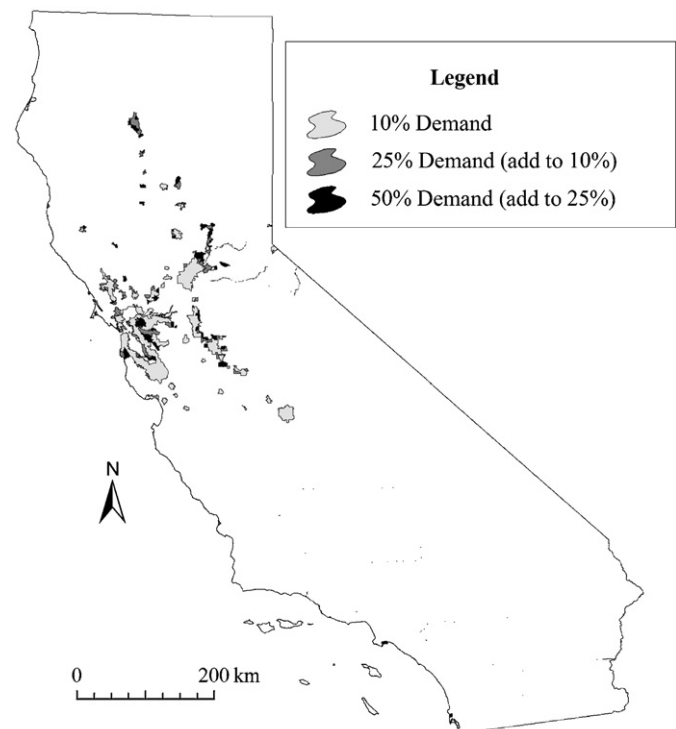


Fig. 6. Hydrogen demand scenarios.

Table 1
Summary of the hydrogen demand scenarios considered

	Total demand (kg/day)	Number of hydrogen vehicles
1% demand scenario	39,090	65,150
10% demand scenario	412,407	687,345
25% demand scenario	994,294	1,657,157
50% demand scenario	2,015,536	3,359,226

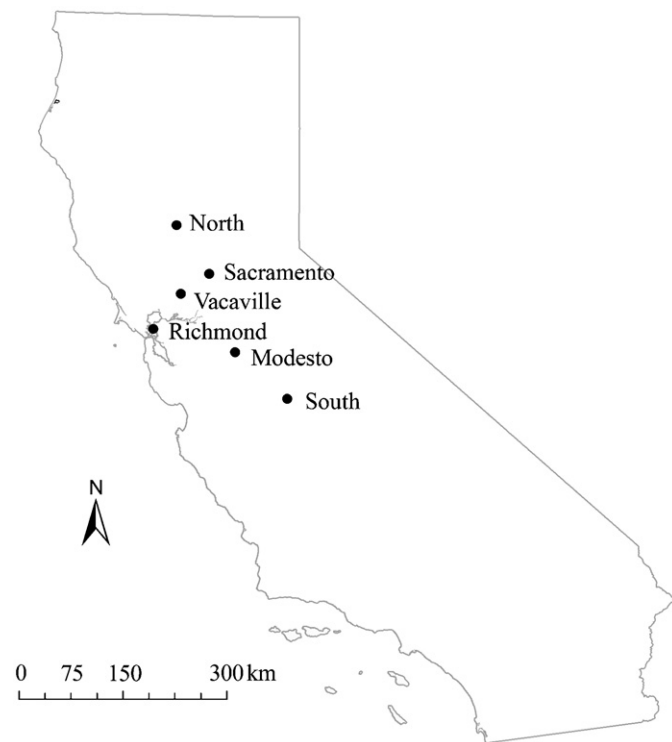


Fig. 7. Possible sites for hydrogen production from rice or wheat straw.

8.2. Cost data

A basic summary of the cost data used in the model is given below. See Parker (2007) for more detailed information.

The delivered cost of the straw feedstock depends on the harvest cost, storage cost, transportation costs and payments to farmers. The costs for both straw feedstocks are based on a study by Jenkins et al. (2000) estimating the cost of rice straw harvest, storage and transport. Fig. 8 shows how the delivered costs of the two feedstocks depend on the delivery distance. Rice straw is more expensive on an energy basis because a ton of rice straw contains less energy than a ton of wheat straw due to higher ash concentration in rice straw. The cost per ton is equal.

As discussed earlier, the literature on hydrogen production from biomass has a wide range of estimates. We model the hydrogen production costs based on Larson et al. (2005). The modeled gasification facility uses the straw feedstock for all process energy needs and co-produces a small quantity of electricity. The conversion process has an efficiency of 63% of the energy in the feedstock converted to hydrogen energy and produces 2.63 kWh of electricity for every kilogram of hydrogen produced. The efficiency is also likely a function of scale such that the amount of electricity per ton hydrogen may vary with scale. However, this was not modeled. The cost function used here is shown in Table 2 along with estimates from other studies.

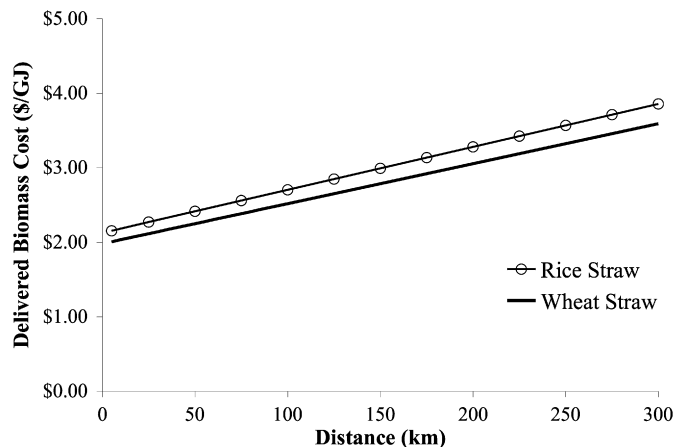


Fig. 8. Delivered cost of biomass feedstock as a function of the delivery distance, rice straw is more expensive to collect and transport because it has a lower energy content compared to wheat straw.

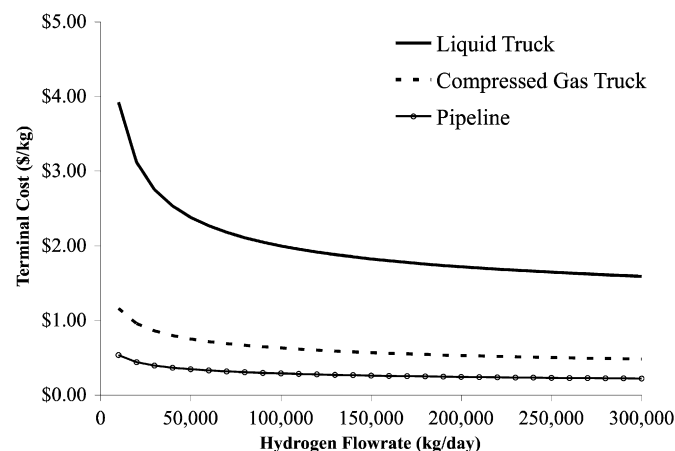


Fig. 9. Levelized cost of hydrogen terminal plotted against the size of the terminal.

Hydrogen distribution incurs costs at three stages. The hydrogen distribution terminal is located at the production facility. The purpose of the distribution terminal is to prepare the hydrogen for delivery through compression or liquefaction depending on the mode of delivery. Buffer storage of hydrogen is also included in the distribution terminal. Hydrogen delivery by trucks or pipelines adds capital and operating costs. Costs are also required at the refueling station to prepare the hydrogen for dispensing into the high-pressure tanks on vehicles. At each of these stages, the costs depend on the mode of delivery, the quantity of hydrogen delivered and the distance of hydrogen delivery. The US Department of Energy’s Hydrogen (H2A) Analysis Model (2007) is the basis for all costs involved in the distribution of hydrogen to the end-users.

Fig. 9 shows the cost added to a kilogram of hydrogen at the distribution terminal for each of the three hydrogen delivery modes with dependence on the size of the terminal. The liquid hydrogen truck mode has the highest costs due to high capital costs and electricity consumption of the liquefier. The pipeline terminal has the lowest costs because it has low compression needs and some of the buffer storage is provided by the pipelines, reducing the storage costs.

Hydrogen delivery by truck depends on the distances between the production facility and the refueling station. The major difference between the two modes of truck delivery is that

compressed gas tube trailers carry only 280 kg of hydrogen per trip while the liquid trucks carry 4142 kg per trip. With the higher payload, each kilogram of hydrogen delivered by a liquid truck must pay a smaller portion of the cost of truck operation compared with a kilogram delivered by a compressed gas truck.

Pipeline delivery of hydrogen requires building a new pipeline network. The pipeline network is modeled to follow the shortest path along the road network for connections between cities and production facilities. Within-city pipeline lengths are determined by an idealized model of the city developed by Yang and Ogden (2007). The idealized city model simplifies within-city delivery distances by assuming the refueling stations are uniformly distributed within a circular city with equal area to the actual city.

The cost of pipelines is assumed to be dependent on the length and location of the pipeline alone. Rural and urban pipelines are differentiated in this work with urban pipelines costing 1.5 times the rural pipeline cost of equal length. The modeled pipeline cost does not depend on the flow rate of hydrogen through the pipeline. The pipe is assumed to be 30 cm diameter. This simplification is supported by analysis showing little difference in installed cost for natural gas pipelines between 15 and 30 cm in diameter (Parker, 2004). It was determined that no booster pumps would be needed given the size of the pipe and the maximum length of the pipeline.

Hydrogen loss during distribution varies substantially between the hydrogen delivery modes. According to the H2A model developed by the Department of Energy (US DOE, 2007), liquid truck delivery loses 8.7% of the hydrogen over the course of distribution, mostly due to losses during liquid hydrogen transfer. Pipeline and compressed gas truck delivery modes lose significantly less hydrogen in the course of delivery.

The cost of the refueling station depends on the mode of hydrogen delivery and the size of the station. Different station sizes are needed to ensure adequate coverage in the different demand scenarios. In the 1% hydrogen demand scenario, the number of stations is at least 10% of current gasoline stations for each demand center, to assure convenient refueling for consumers. This increases to 50% of current gasoline stations in the 50% hydrogen demand scenario. The coverage requirement determines the station size for each scenario. Fig. 10 shows the costs used in this study for each mode of delivery and for the station sizes of each demand scenario. Station costs are adapted from the US Department of Energy's H2A model (US DOE, 2007). The compressed gas truck refueling station is limited to stations smaller than 560 kg/day due to logistical difficulties for more than

two truck deliveries per day. In the 25% and 50% demand scenarios compressed gas truck stations are 560 kg/day.

8.3. Greenhouse gas emissions data

Greenhouse gas emissions occur in a number of stages along the supply chain. Emissions included in this analysis are from the increased use of fertilizers, the burning of diesel fuel and the consumption of electricity. Harvesting biomass causes emissions through the combustion of diesel by the farm equipment. Removing residue biomass from agricultural fields also strips nutrients that would otherwise replenish the soil. Those nutrients may need to be replaced through fertilizers if not replaced by return of ash to the fields, thus producing more emissions. Nitrogen is the primary nutrient to be replaced as it is volatilized during gasification (Yomogida and Jenkins, 1997). Biomass delivery consumes more diesel fuel. Emission factors associated with unit use of these activities are given in Table 4. These unit emission rates are constant. Diesel consumption is calculated for both harvest and transportation using the engineering-economic models detailed in Parker (2007). Fertilizer use associated with residue removal is computed using methods adopted from Yomogida and Jenkins (1997). Electricity usages associated with hydrogen production and hydrogen distribution are given in Tables 2 and 3.

No direct emissions are considered as coming from the production facility since all carbon released originated from the growing of biomass, which takes the carbon out of the atmosphere. Power supplied from fossil sources to the facility results in net greenhouse gas emissions if the co-product electricity is insufficient to meet the full needs. Hydrogen distribution produces emissions through the use of electricity in compression or liquefaction of hydrogen and the combustion of diesel by the delivery trucks. The electricity produced at the biomass facility is consumed before any grid electricity so that the net electricity consumption of the supply is used in calculation of electricity emissions. The analysis assumes the replacement or consumption of natural gas combined-cycle produced electricity, which is consistent with California's regulations on future electric generation in the state.

9. Results

In this section, we present results from the 8 case studies described above, identifying the optimal system design, the capital cost of the system, the delivered hydrogen cost, and the greenhouse gas emissions. We found that in many of the cases hydrogen from biomass is cost competitive with fossil hydrogen while providing significant reductions in greenhouse gas emissions.

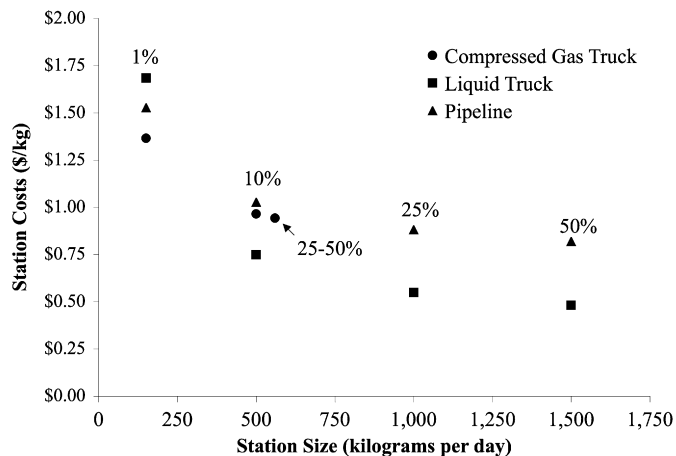


Fig. 10. Levelized cost of hydrogen refueling stations.

Table 2
Economics and performance of gasification facility

Parameter	Value
Capital cost ^a	\$991,166x ^{0.712}
Fixed operating cost	5% of total capital per year
Variable operating cost	\$1.85 per ton straw consumed
Hydrogen efficiency	63% HHV
Rice straw	74.1 kg H ₂ /dry ton
Wheat straw	77.7 kg H ₂ /dry ton
Electricity production	2.63 kWh/kg H ₂

^a x is the capacity of the gasification facility in dry tones of straw per year.

Table 3
Summary of hydrogen delivery modes

Delivery mode	Electricity use (kWh/kg)	Hydrogen losses (%) ^a	Truck payload (kg)
Compressed gas truck	2.02	1	280.3
Liquid truck	11.05	8.7	4142
Pipeline	2.76	1.5	–

^a Losses derived from the cumulative losses over the distribution system as reported in the H2A model (US DOE, 2007).

Table 4
Greenhouse gas emission factors

	Emission factors
Diesel combustion	3500 g CO ₂ -eq/l diesel ^a
Electricity use	500 g CO ₂ -eq/kWh ^b
Fertilizer use	42 kg CO ₂ -eq/ton straw removed ^c

^a Based on GREET 1.7a (ANL, 2007).

^b Emissions for natural gas combined cycle electricity from GREET 1.7a (ANL, 2007).

^c Nutrient replacement requirements taken from Yomogida and Jenkins (1997), emissions calculated using GREET 1.7a (ANL, 2007).

Table 5
Optimal biomass hydrogen production sites and delivery modes

	Feedstock	
	Rice straw	Wheat straw
Hydrogen demand	1%	Vacaville
	10%	<i>Sacramento</i>
	25%	<i>Richmond</i>
	50%	<i>Sacramento</i>
		<i>Richmond</i>

Italic = compressed gas truck delivery.
Bold italic = pipeline delivery.

9.1. Optimal system design

In all scenarios considered, designs with a single production facility give the lowest cost. The two lowest hydrogen demand scenarios (1%, 10%) found compressed gas truck delivery of hydrogen to be least-cost and the optimal layout sited the conversion facility near the demand to minimize the cost of hydrogen delivery. The optimal design for the higher hydrogen demand scenarios (25%, 50%) used pipeline delivery of hydrogen and also sited the facilities near large demand centers to minimize pipeline lengths. Sacramento appears as the optimal site in a number of cases as it is both a large demand center and relatively close to the major biomass resources. The design results for our eight cases are summarized in Table 5, which shows the least-cost delivery mode, and the optimal site for the hydrogen plant for each case. The optimal system design for the 10% demand/wheat straw scenario is shown in Fig. 11 as an example of the optimal spatial layout for the supply chain.

Locating the hydrogen production facility represents a tradeoff between feedstock transportation costs and hydrogen fuel transportation costs. In general, incremental costs of hydrogen delivery by compressed gas truck or pipeline (from the production plant to refueling stations) is more expensive than biomass delivery (from the field to the production site) while the opposite is true for liquid truck delivery of hydrogen. As a result, hydrogen production facilities are located to minimize hydrogen delivery distances in systems where compressed gas truck or pipeline delivery of hydrogen provides the lowest system cost. For this reason, all the hydrogen production facilities in the case studies are located near large demand centers. In contrast, biomass hydrogen systems using liquid truck delivery locate the production facility to minimize feedstock delivery distances. The uncertain result of this tradeoff highlights the importance of systems analysis for designing the biomass hydrogen supply chain.

9.2. System costs

Hydrogen delivery, including terminal, distribution, and station costs, is a major contributor to the delivered cost of hydrogen from biomass resources. Fig. 12 shows the contribution of each

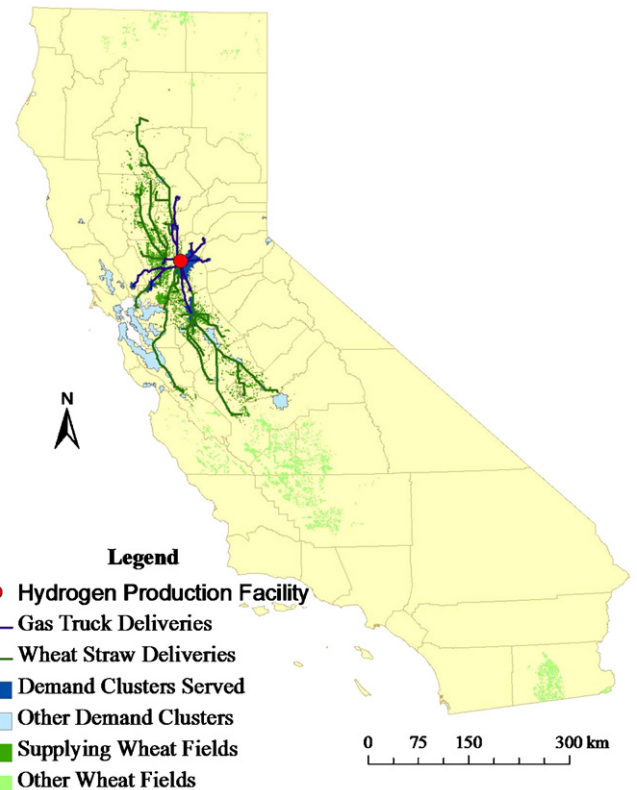


Fig. 11. Optimal system design for the scenario with wheat straw and 10% hydrogen demand, showing optimal facility location, wheat straw deliveries and compressed gas truck hydrogen deliveries.

stage of the biomass hydrogen supply chain to the delivered cost of a kilogram of hydrogen for the lowest cost supply chains for each scenario. In low demand scenarios, hydrogen delivery is twice as expensive as the production of hydrogen including the feedstock costs. At higher demands the production and delivery costs are approximately equal.

In Table 6, we show the hydrogen selling prices needed to induce investment in biomass hydrogen infrastructure. Recall that biomass is in competition for the hydrogen market with other sources and will only be used if biomass can be produced below the given selling price. For example, for hydrogen from rice straw at 10% hydrogen demand, a selling price of \$4.09/kg would be required for the biomass hydrogen system to be competitive. Selling prices needed to induce investment in biomass hydrogen infrastructure decline sharply between the 1% and 10% demand scenarios. With hydrogen demands of 25% and 50% of the light-duty vehicle fleet, the cost of hydrogen from the two straw resources becomes competitive with some fossil sources of hydrogen (see Fig. 13). It is important to note that biomass supplies only a fraction of the hydrogen in the higher scenarios. The cost improvements between the 10% and 50% demand scenarios result from denser hydrogen demands leading to lower distribution costs. The feedstock and production costs do not change.

The biomass feedstock costs resulting from optimal system design are significantly higher than the assumed feedstock costs in all gasification studies in the literature (Hamelinck and Faaij, 2002; Larson et al., 2005; Lau et al., 2003; NRC, 2004; Simbeck and Chang, 2002; Spath et al., 2003, 2005). Lower feedstock costs could be achieved at different sites or with smaller conversion facility sizes. However, designs that simply minimize feedstock costs are not optimal from a total system perspective. The higher feedstock costs here are offset by lowering the hydrogen delivery cost resulting in lower total costs.

Furthermore, rather than multiple hydrogen production facilities at multiple demand centers, the optimal solution from the model suggests a single facility. Considering feedstock and

hydrogen production costs alone, the optimal facility size is much smaller than when considering the full system. This is due to the economies of scale in the hydrogen distribution terminals. Hydrogen compressors and liquefiers have strong scaling factors of 0.52 and 0.67, respectively, in the cost functions used here. These economies of scale push the system toward larger hydrogen production facilities and terminals.

9.3. Supply curve analysis

We find that the least-cost biomass hydrogen supply chains do not utilize the full biomass supply. However, at higher selling prices it becomes profitable to utilize more and more of the biomass supply until the maximum supply is reached. Supply curves show how the quantity of hydrogen available from biomass varies with hydrogen selling price. The curves represent the quantity of hydrogen that would be produced from the straws at various hydrogen selling prices for the eight scenarios. Each time the quantity of hydrogen supplied changes along the curve, this represents a different optimal configuration for the entire system. Where the supply curve is flat represents a profit-taking region for the hydrogen supplier maintaining the same optimal configuration.

For reference, the cost ranges for comparable onsite steam methane reformer stations are included on the supply curve charts. Current and future technology costs are adapted from the National Academies report (2004). Cost ranges were calculated based on natural gas prices of \$5.11 per MMBtu to \$10.13 per MMBtu. These prices represent the 10th lowest and 10th highest monthly average commercial natural gas prices in California for the period January 2000–November 2010 according to the Energy Information Administration (2007). Separate supply curves were developed for each demand scenario. The demand scenarios play a role in determining the prices in the supply curve by determining the hydrogen distribution system needed. More dense demands have lower distribution costs, shifting the supply curves to the left compared with less-dense demands.

For the 10% hydrogen demand scenario shown in Table 6, rice straw-based hydrogen requires a price just above \$4/kg to come to market. Nearly all the rice straw is used in this supply configuration. Wheat straw-based hydrogen comes into the market at a higher price and with a lower supply that gradually increases to the maximum as the price is increased. The full wheat straw resource would not be utilized unless the price of hydrogen is greater than \$5/kg. At higher demands, biomass hydrogen moves from being competitive with current technology onsite SMRs to being competitive with future technology onsite SMRs. This result means that biomass hydrogen is likely to compete with onsite SMRs throughout a transition to hydrogen-fueled transportation sector. For another point of comparison, producing hydrogen at the refueling station through electrolysis of wind and

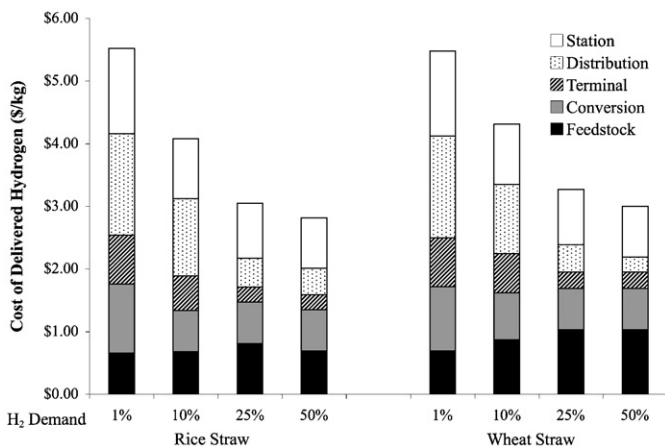


Fig. 12. Contribution to the delivered cost of biomass hydrogen for each component of the system.

Table 6
Summary of results for optimal market-entry biomass supply chains

Hydrogen demand:	1%		10%		25%		50%	
	Rice	Wheat	Rice	Wheat	Rice	Wheat	Rice	Wheat
Required H ₂ selling price (\$/kg)	5.53	5.49	4.09	4.32	3.40	3.63	2.98	3.27
Feedstock cost (\$/GJ)	2.88	3.05	2.94	3.84	3.49	4.48	3.00	4.48
Capital cost per vehicle served by biomass (\$)	4100	4025	2730	2920	1900	3020	1865	2580
Conversion facility size (kg/day)	43,871	43,871	182,502	105,883	186,433	160,239	186,433	160,239
# Vehicles served by biomass	65,389	65,389	272,015	157,816	276,479	237,633	276,479	237,633
% of H ₂ produced from biomass	100	100	39	23	17	14	8	7

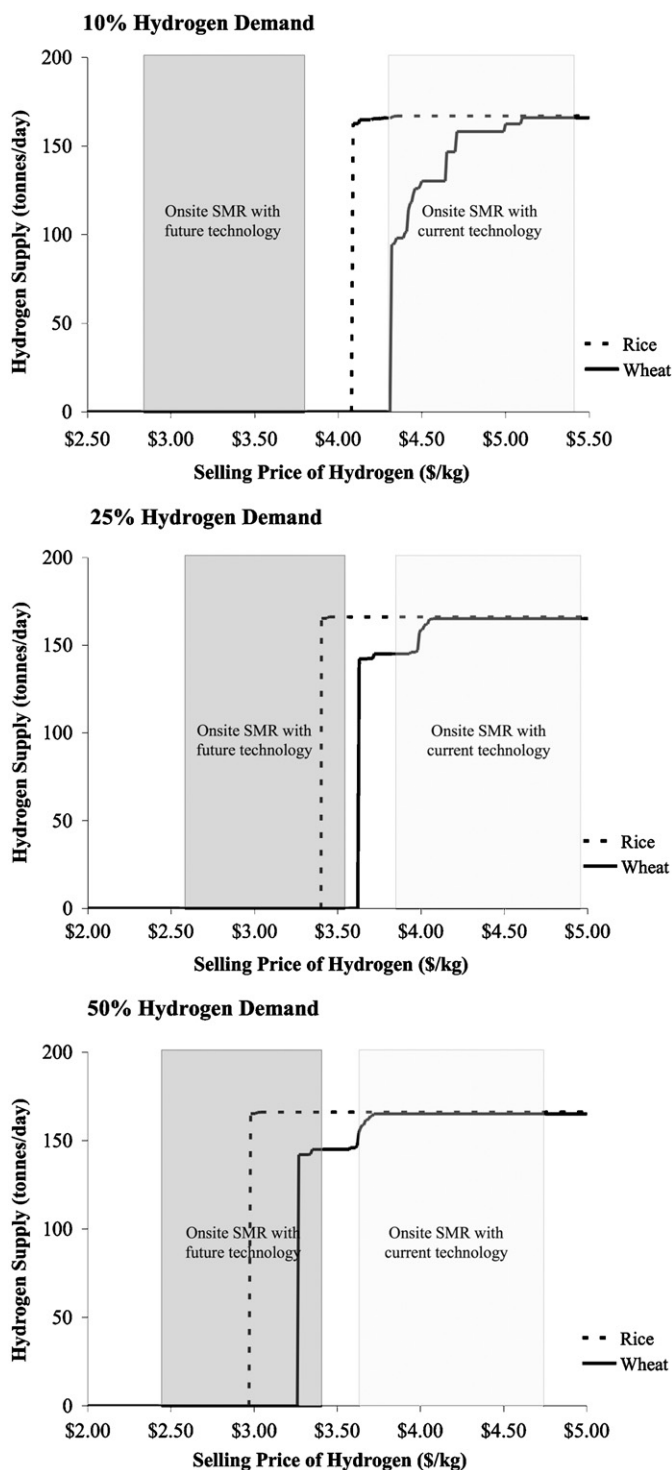


Fig. 13. Supply curves for hydrogen from rice or wheat straw for scenarios of 10%, 25%, and 50% hydrogen demand; the axis are opposite of traditional supply curves with price on the horizontal axis.

solar energy is estimated at \$10.69 and \$28.19/kg, respectively with current technology dropping dramatically to \$2.86 and \$6.18/kg with future technology (NRC, 2004).

9.4. Robustness of results

Sensitivity analysis was performed on the economic parameters expected to have the largest impact on the cost and system

design. These sensitivity parameters include both the technical specifications of the system such as gasifier efficiency as well as indicators of the larger economic context such as electricity prices. Table 7 lists the sensitivity parameters tested along with their ranges.

The delivered cost of hydrogen did not vary more than 50 cents/kg of hydrogen (11%) with the given bounds of sensitivity analysis. The internal rate of return had the largest impact of the parameters reflecting the capital intensity of the system. Also important are the gasifier capital costs, pipeline capital costs, feedstock costs, and efficiency (Fig. 14).

We found that the price of electricity and the capital cost of pipelines have the largest impact in terms of changing the system design. Lowering electricity prices from 9 to 5.5 cents/kWh switched both the 10% and 25% hydrogen demand scenarios to liquid hydrogen delivery with facilities located to minimize feedstock costs. Increasing or decreasing the capital costs of pipelines varies the level of hydrogen demand needed to make pipelines a viable delivery mode.

9.5. Greenhouse gas emissions

The well-to-wheel greenhouse gas emissions of hydrogen produced from rice straw and wheat straw are significantly lower than both conventional gasoline and hydrogen produced from natural gas. The emissions include the operation of equipment to harvest and deliver the straw, fertilizers required to replace nutrients removed from the soil, and the diesel and electricity used in hydrogen distribution. No greenhouse gas emissions other than water are expected for the operation of a fuel cell vehicle.

The systems designed for achieving economic optimality produce greenhouse gas emissions less than a tenth of conventional gasoline vehicles. This improvement far outpaces gains possible from advanced gasoline hybrid vehicles. The especially low emissions results in the cases shown here are due to the choice of gaseous truck or pipeline modes for hydrogen delivery. A net gain of renewable electricity results from the gaseous truck delivery mode while the pipeline mode results in only a small net consumption of grid electricity. Significantly higher electricity use in the liquid truck hydrogen delivery mode results in emissions of 5425 g CO₂-eq/kg of hydrogen or 3 times the emissions of the same hydrogen delivered by gaseous truck but still less than half the emissions of hydrogen from onsite SMR (Fig. 15).

Including a value for carbon will make biomass hydrogen more attractive relative to natural gas-based hydrogen. The economic analysis showed that biomass hydrogen could be produced at costs in the range of natural gas hydrogen costs. For every \$10 per ton increase in the value of carbon dioxide, the cost difference between biomass and natural gas hydrogen will be reduced by about ten cents per kilogram of hydrogen.

10. Discussion

In our case study of California, the available biomass waste resource can fuel approximately 40% of the current light-duty vehicle fleet with hydrogen. This is a significant potential in-state resource for renewable transportation fuel. This estimate depends on using all the technically available biomass wastes for hydrogen production, and assumes an efficient (51.5 mile per gallon equivalent) hydrogen fuel cell car. While not all the technically available resource is likely to be exploited for hydrogen, it highlights that biomass could become a major hydrogen resource.

We found that the cost of biomass hydrogen is potentially competitive with fossil hydrogen sources for an optimally designed biomass hydrogen supply chain. It appears that biomass

Table 7
Parameters for sensitivity analysis

Parameter	High value	Base case	Low value
Feedstock harvest cost	+90%	\$15.95/dry ton	−40%
Gasifier capital cost	+30%	\$185 million for 100,000 kg/day	−30%
Pipeline capital cost (\$/mile)	\$1,230,680	\$615,340	\$461,505
	\$1,846,020	\$923,010	\$692,258
Gasifier efficiency	65%	63%	51%
Electricity price	\$0.11/kWh	\$0.09/kWh	\$0.055/kWh
Diesel price	\$3.50/gal	\$2.50/gal	\$1.50/gal
Internal rate of return	15%	10%	5%
Gasifier capacity factor	0.95	0.9	0.8

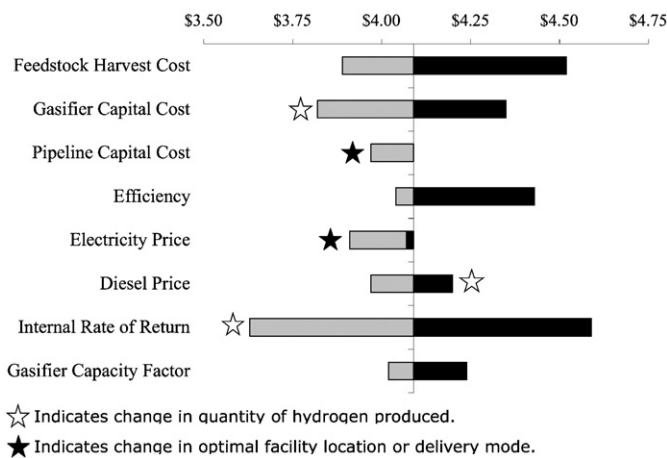


Fig. 14. Sensitivity analysis for scenario with rice straw and 10% hydrogen demand; the center line represents the base case cost.

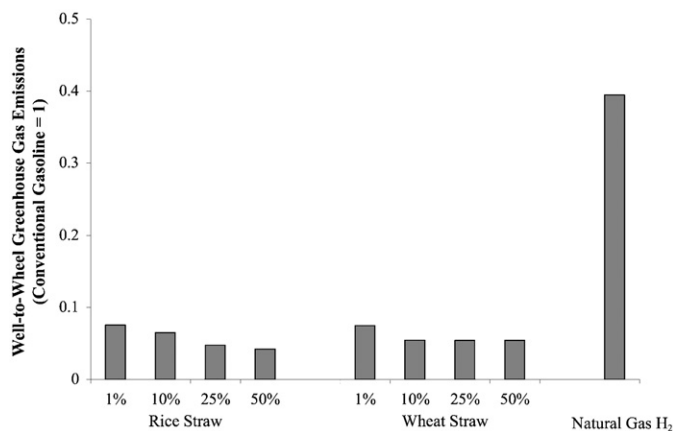


Fig. 15. Well-to-wheels greenhouse gas emissions for economically optimal system designs.

hydrogen could offer low-cost renewable hydrogen significantly lower than current technology wind and solar and similar to future technology wind hydrogen. The price premium for biomass hydrogen compared with on-site natural gas SMR-based hydrogen was less than \$1/kg for the case studies we performed (comparing low demand scenarios with current technology and high demand scenarios with future technology). Similar or even better results might be possible with other biomass waste feedstocks in California, as rice straw and wheat straw are not exceptionally low-cost wastes. The results found here will translate best for other regions, such as the upper Midwest US,

with large agricultural waste streams and significant population centers.

Achieving low costs requires clever system design. Throughout our analysis, we found that with biomass hydrogen it is critically important to optimize the entire supply chain. Optimizing a portion of the supply chain will not accomplish the task. By performing a full supply chain optimization, we gain a better understanding of the many tradeoffs involved in delivering biomass hydrogen at a low cost. For instance, simply minimizing the cost of producing biomass hydrogen without considering hydrogen delivery can lead to expensive biomass hydrogen. The high cost of hydrogen distribution mandated locating and sizing the facility near the demand. It costs more to produce hydrogen when the hydrogen plant is far from the field, but much less to deliver hydrogen to users. Second, we found that single large facilities are preferred, at least in the cases examined.

There are clear carbon reduction benefits from biomass hydrogen, as compared to other near-term fossil competitors. For the scenarios we investigated biomass hydrogen provided hydrogen energy to vehicles with only about one-fifth of the greenhouse gas emissions as providing that same hydrogen from natural gas steam methane reforming.

Our study has implications for both hydrogen policy and R & D priorities. Biomass hydrogen was assessed to have a poor-to-mediocre outlook in the recent National Academies study on hydrogen (NRC, 2004) leading to reduced funding from the United States Department of Energy. The NAS study suggested that hydrogen from small steam methane reformers would be more promising than renewable sources, including biomass, for a long time into the future. We found that this view of biomass hydrogen is in many respects due to the non-optimal system design assumptions for NAS's biomass hydrogen supply system. For example, the NAS study assumed that only energy crops were used (instead of lower cost biomass wastes), and that the hydrogen plant was small (having poor-scale economy) and had a low conversion efficiency.

In reviewing other recent literature on biomass hydrogen, and taking a systems design view, we found that the picture for biomass hydrogen is both more complex and more promising. Applying system integration and optimization, we showed that biomass hydrogen can potentially compete with the near-term option of natural gas steam reforming at the refueling station in California. Biomass also has the benefit of low greenhouse gas emissions. It may produce less than one fifth the greenhouse gas emissions as steam methane reforming. With this knowledge, our view is that biomass-based hydrogen can be a cost competitive low-carbon source of transportation fuel in the near- to mid-term. It is clear that biomass hydrogen deserves serious further consideration and research.

We plan to further this work by developing models for the supply chains of other transportation fuels that would utilize biomass resources and expand the number and scope of resources

considered in order to explore the best use of feedstock for transportation fuels. We also plan to pursue methodological improvements that will allow us to analyze both the uncertainty of supply and demand and the dynamics of growth for biomass-based fueling infrastructures.

11. Conclusion

The resource base exists for waste biomass hydrogen to play a significant role in the future transportation energy needs of California. The cost of biomass hydrogen can be competitive with fossil sources of hydrogen, especially in cases with high hydrogen demand density with a dense resource supply nearby. There is a marked improvement in greenhouse gas emissions from the waste biomass hydrogen systems considered here and either natural gas-based hydrogen or conventional gasoline. Finally, we found that the competitiveness of biomass hydrogen will depend on a full systems design approach to the supply chain.

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Appendix

A.1. Model notation

subscript i refers to different fields
 subscript j refers to different potential conversion sites
 subscript k refers to different hydrogen demand clusters
 subscript m refers to different modes of hydrogen delivery
Inputs:

$feedstock_yield_i$ feedstock available at field i (tons/year)
 P_k selling price of demand at cluster k (\$/kg)
 $daily_demand_k$ demand at cluster k (kg/day)
 α_q scaling factor for various technologies
 f_{2H} hydrogen per ton of rice straw (kg/ton)
 f_loss loss factor accounting for feedstock losses in storage and transport
 t_loss^m loss factor accounting for hydrogen losses at a terminal of mode m
 d_loss^m loss factor for hydrogen losses in the distribution system of mode m
 d_{ij} distance between field i and site j (km)
 d_{jk} distance between site j and demand cluster k (km)
Decision variables:
 F_{ij} yearly quantity of feedstock delivered from supply node i to conversion site j (mg/year)

C_j capacity of conversion facility at site j (kg H₂/day)
 T_j^m capacity of hydrogen terminal of mode m at site j (kg H₂/day)
 H_{jk}^m capacity of hydrogen delivery link by mode m from site j to demand cluster k (kg H₂/per day)
 Hb_{jk} binary variable for the existence of pipeline link between site j and cluster k
 $I_{k_1k_2}$ capacity of pipeline link between demand clusters k_1 and k_2 (kg H₂/day)
 $Ib_{k_1k_2}$ binary variable for the existence of pipeline link between clusters k_1 and k_2
 S_k^m hydrogen supply capacity for demand cluster k by mode m (kg H₂/per day)
Intermediate variables:
 FC_{ij} cost of feedstock delivered from field i to site j (\$/year)
 CC_j conversion cost at site j (\$/year)
 TC_j^m terminal cost at site j for hydrogen delivery mode m (\$/year)
 DC_{jk}^m delivery costs from site j to cluster k by mode m (\$/year)
 $IC_{k_1k_2}$ intercity pipeline delivery costs between clusters k_1 and k_2 (\$/year)
 LC_k^m local delivery cost within cluster k by mode m (\$/year)
 RC_k^m refueling station costs for cluster k for stations receiving hydrogen by mode m (\$/year)
 X_k yearly quantity of hydrogen sold at demand cluster k (kg/year)

A.2. The equations

The optimization model consists of an objective function and a set of constraints. The objective function defines the variable of interest and the desired value for the variable. In this case the variable is profit and the desired value is as large as possible. The constraints define the reality of the system in question. They ensure that the abstract math in the model corresponds to some reality. The following is the formulation used in the optimization model with explanations as to the meaning of each equation.

A.2.1. The objective

The objective is to build an industry that will maximize profit with given demands, supplies, and prices. The objective function is the profit function of annual revenue, price multiplied by annual quantity of hydrogen sold, minus annualized cost of production

$$\begin{aligned} \text{Maximize } \pi &= \sum_k P_k X_k - \text{annualized_cost} \\ \text{annualized_cost} &= \sum_{i,j} FC_{ij}(F_{ij}, d_{ij}) + \sum_j CC_j(C_j) \\ &+ \sum_{m,j} TC_j^m(T_j^m) + \sum_{j,k,m} DC_{jk}^m(H_{jk}^m, d_{jk}) \\ &+ \sum_{k_1,k_2} IC_{k_1k_2}(I_{k_1k_2}, d_{k_1k_2}) + \sum_{m,k} LC_k^m(S_k^m) + \sum_k RC_k^m(S_k^m) \end{aligned} \quad (\text{A.1})$$

The annualized cost of production will depend on the capacities of the infrastructure built (C_j , T_j^m , S_k^m , H_{jk}^m , and I_{kk}) as well as quantities delivered/produced/converted at each node and along each link. In the formulation of this model, the quantities delivered/produced/converted on each link or at each node are assumed to be a constant fraction of the installed capacity this fraction is denoted by the capacity factor.

The cost functions are where the need for non-linear and binary variables arose in this problem. Binary variables are integer variables that take on only the values one or zero. They are not

continuous, which makes them computationally difficult. The following equations give the general form of cost functions for the different components of the supply chain. Attention should be paid to where the model is forced to use non-linear and binary variables in order to accurately replicate the cost functions. The equations shown here give a general description of the problem.

The feedstock cost has fixed costs of harvest, storage, and truck loading/unloading per ton of feedstock and a variable cost that is linearly dependent on the delivery distance

$$FC_{ij}(F_{ij}, d_{ij}) = (\text{harvest_cost}_i + \text{storage_cost}_i + \text{delivery_cost}_{ij}(d_{ij}))F_{ij} \quad (\text{A.2})$$

The conversion cost (CC_j) represents the capital and operating costs of the conversion facility. The capital cost is a nonlinear function dependent on the capacity. The yearly charge paid on the capital is the capital recovery factor (CRF in the equation) multiplied by the total installed cost of capital. Fixed operating costs can be simplified as a multiplier of the capital costs (O&M in the equation). The rest of the operating costs are linear functions of the quantity produced which equals the capacity multiplied by the capacity factor (CF)

$$CC_j(C_j) = (\text{CRF} + O \& M)\text{cap_cost}C_j^2 + \sum_q \text{variable_cost}_q C_j CF \quad (\text{A.3})$$

A second cost is added to the supply chain at the conversion facility. The cost of preparing the product hydrogen for transport to the refueling stations is the terminal cost (TC_j^m). The terminal cost has components that are nonlinear in capacity representing the capital and fixed operating cost for the terminal equipment. There are also linear components for the variable cost such as electricity. Each facility has three possible types of terminals and can even have two different types at the same facility

$$TC_j^m(T_j^m) = \sum_q (\text{CRF}_q + O \& M_q)\text{cap_cost}_q(T_j^m)^{z_q} + \sum_q \text{variable_cost}_q T_j^m CF \quad (\text{A.4})$$

The delivery costs must be broken into pipeline and truck delivery cost as the two have different forms to their cost equations. The two truck modes follow a linear function of capital and operating cost associated with the truck cab, trailer, and driver salary. There are also per mile costs associated with fuel, maintenance, and insurance. Truck transmission costs have the form shown in Eq. (A.5)

$$DC_{jk}^{m=\text{gas,liq}}(H_{jk}^m, d_{jk}) = (\text{CRF}_{cab} + O \& M_{cab})\text{cap_cost}_{cab}(\#cabs(H_{jk}^m)) + \text{driver_salary}(\#cabs(H_{jk}^m)) + (\text{CRF}_{tr} + O \& M_{tr})\text{cap_cost}_{tr}^m(\#trailers) + \text{per_mile}^m H_{jk}^m d_{jk} \quad (\text{A.5})$$

The pipeline costs are only capital and fixed operating and maintenance cost because compression is included in the terminal cost. Pipeline costs are treated with binary variables of whether a pipeline is on a link or not with a constant per kilometer cost. Intercity and intracity pipelines are differentiated in costs with the intracity pipelines costing 1.5 times more than the intercity pipelines

$$DC_{jk}^{m=\text{pipe}}(Hb_{jk}, d_{jk}) = (\text{CRF} + O \& M)\text{cap_cost}Hb_{jk}d_{jk} \quad (\text{A.6})$$

For pipelines there are also deliveries taking place between cities. These intercity deliveries are represented by the following:

$$IC_{k_1 k_2}(Ib_{k_1 k_2}, d_{k_1 k_2}) = (\text{CRF} + O \& M)\text{cap_cost}Ib_{k_1 k_2} d_{k_1 k_2} \quad (\text{A.7})$$

The local delivery costs follow the same form as transmission costs except that the distances are determined by the idealized city model.

Refueling station costs are different for each mode. The capital costs and fixed operations and maintenance are nonlinear functions of the capacity and linear variable costs also exist

$$RC_k^m(S_k^m) = \sum_q (\text{CRF}_q + O \& M_q)\text{cap_cost}_q(S_k^m)^{z_q} + \sum_q \text{variable_cost}_q S_k^m CF \quad (\text{A.8})$$

A.2.2. The constraints

In order to model reality, constraints need to be imposed on the objective function. Without constraints, the model would sell infinite amounts of hydrogen while building negative capacity leading to an infinite amount of profit. The constraints can be placed into three categories; capacity constraints, flow constraints, and non-negativity constraints. The capacity constraints restrict quantities to be less than the maximum allowed by the built or given capacities. Flow constraints require that at each node the quantities going in must equal the quantities going out plus or minus the quantities supplied or consumed at the node. Non-negativity constraints require that all physical quantities be positive as they cannot be negative.

A.2.2.1. Capacity constraints. The feedstock extracted from a field must be less than or equal to the feedstock yield of that field

$$\sum_j F_{ij} \leq \text{feedstock_yield}_i \quad (\text{A.9})$$

The yearly capacity of a conversion facility (C_j) must be greater than the hydrogen production potential of the feedstock coming into the conversion facility (F_{ij}). The f_{2H} multiplier converts feedstock quantity into equivalent hydrogen production capacity. The f_{loss} multiplier accounts for feedstock loss in storage and transport

$$\sum_i f_{loss} F_{ij} f_{2H} \leq 365 C F C_j \quad (\text{A.10})$$

The capacity of the terminals (T_j^m) at a conversion facility needs to equal the capacity of the conversion facility (C_j)

$$\sum_m T_j^m = C_j \quad (\text{A.11})$$

The capacity of the terminal of a mode at a conversion facility (T_j^m) must be greater than the hydrogen leaving the conversion facility by that mode (H_{jk}^m)

$$\sum_k H_{jk}^m \leq t_{loss}^m T_j^m \quad (\text{A.12})$$

The capacity of the gas truck or liquid truck local distribution and refueling infrastructure ($S_k^{\text{gas,liquid}}$) must be at least as large as the quantity of hydrogen coming into a demand center by gas truck or liquid truck

$$\sum_j d_{loss}^{\text{gas,liquid}} H_{jk}^{\text{gas,liquid}} \leq S_k^{\text{gas,liquid}} \quad (\text{A.13})$$

The capacity of the local pipeline distribution and refueling infrastructure (S_k^{pipe}) must be greater than the net hydrogen coming into the demand center

$$\sum_j d_{loss}^{\text{pipe}} H_{jk}^{\text{pipe}} + \sum_{k_2} I_{k_2 k} - \sum_{k_2} I_{k k_2} \leq S_k^{\text{pipe}} \quad (\text{A.14})$$

The capacity of the local distribution and refueling infrastructure at a demand center must be greater than the amount of

hydrogen sold at the demand center (X_k)

$$X_k \leq \sum_m 365CF_k^m \tag{A.15}$$

The amount of hydrogen sold at a demand center cannot be more than the hydrogen demanded at that center

$$X_k \leq \text{daily_demand}_k 365 \tag{A.16}$$

A.2.2.2. Flow constraints. The hydrogen that can be produced from the feedstock going into the conversion facility must equal the hydrogen coming out of the conversion facility. The H_b variable is a binary variable that is one if a pipeline exists and zero otherwise. This variable allows the pipeline costs to be a constant if a pipeline is built and zero otherwise

$$\sum_i f_{loss} F_{ij} f_{2H} = \sum_k H_{jk}^{gas} / t_{loss}^{gas} + \sum_k H_{jk}^{liquid} / t_{loss}^{liquid} + \sum_k H_b H_{jk}^{pipe} / t_{loss}^{pipe} \tag{A.17}$$

The net hydrogen coming into a demand center must be consumed. I_b is a binary variable for the existence of a pipeline on link $k_1 k_2$

$$\sum_j d_{loss}^{gas} H_{jk}^{gas} + \sum_j d_{loss}^{liquid} H_{jk}^{liquid} + \sum_j d_{loss}^{pipe} H_b H_{jk}^{pipe} + \sum_{k_2} I_{k_2 k} I_{k_2 k} - \sum_{k_2} I_{k k_2} I_{k k_2} = X_k \tag{A.18}$$

A.2.2.3. Non-negativity constraints. All capacities and delivered quantities must have zero or positive values

$$X_k, F_{ij}, C_j, T_j^m, H_{jk}^m, I_{k_1 k_2}, S_k^m \geq 0 \tag{A.19}$$

Combining the constraints and the objective function gives a mixed-integer, non-linear program that requires a global solving algorithm. Due to non-convexity of the problem local optimality will not guarantee global optimality. Global solving algorithms are computationally expensive as more of the solution space must be searched to ensure an optimal solution compared with local algorithms. What this means practically is that it is beneficial to provide the solution algorithm as small a problem as feasible while retaining the solution space that will contain the optimal solution.

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