



Technical Breakthrough Points and Opportunities in Transition Scenarios for Hydrogen as Vehicular Fuel

V. Diakov and M. Ruth
National Renewable Energy Laboratory

B. James, J. Perez, and A. Spisak
Directed Technologies, Inc.

NREL is a national laboratory of the U.S. Department of Energy, Office of Energy Efficiency & Renewable Energy, operated by the Alliance for Sustainable Energy, LLC.

Technical Report
NREL/TP-6A10-53489
December 2011

Contract No. DE-AC36-08GO28308

Technical Breakthrough Points and Opportunities in Transition Scenarios for Hydrogen as Vehicular Fuel

V. Diakov and M. Ruth
National Renewable Energy Laboratory

B. James, J. Perez, and A. Spisak
Directed Technologies, Inc.

Prepared under Task No. HS07.1002, EFGH.2000

NREL is a national laboratory of the U.S. Department of Energy, Office of Energy Efficiency & Renewable Energy, operated by the Alliance for Sustainable Energy, LLC.

NOTICE

This report was prepared as an account of work sponsored by an agency of the United States government. Neither the United States government nor any agency thereof, nor any of their employees, makes any warranty, express or implied, or assumes any legal liability or responsibility for the accuracy, completeness, or usefulness of any information, apparatus, product, or process disclosed, or represents that its use would not infringe privately owned rights. Reference herein to any specific commercial product, process, or service by trade name, trademark, manufacturer, or otherwise does not necessarily constitute or imply its endorsement, recommendation, or favoring by the United States government or any agency thereof. The views and opinions of authors expressed herein do not necessarily state or reflect those of the United States government or any agency thereof.

Available electronically at <http://www.osti.gov/bridge>

Available for a processing fee to U.S. Department of Energy and its contractors, in paper, from:

U.S. Department of Energy
Office of Scientific and Technical Information
P.O. Box 62
Oak Ridge, TN 37831-0062
phone: 865.576.8401
fax: 865.576.5728
email: <mailto:reports@adonis.osti.gov>

Available for sale to the public, in paper, from:

U.S. Department of Commerce
National Technical Information Service
5285 Port Royal Road
Springfield, VA 22161
phone: 800.553.6847
fax: 703.605.6900
email: orders@ntis.fedworld.gov
online ordering: <http://www.ntis.gov/help/ordermethods.aspx>

Cover Photos: (left to right) PIX 16416, PIX 17423, PIX 16560, PIX 17613, PIX 17436, PIX 17721



Printed on paper containing at least 50% wastepaper, including 10% post consumer waste.

Table of contents

Table of contents.....	iii
Figures and tables.....	iv
Summary.....	1
Introduction.....	4
Macro-systems model (MSM)	4
HyPro: a hydrogen pathways progression analysis model.....	4
Analysis goals.....	4
Approach	5
Generic hydrogen pathways evolution scenario.....	5
Model assumptions and inputs	5
Hydrogen pathways evolution: generic case.....	8
Greenhouse gas emissions mitigation.....	13
Base case hydrogen pathways with the onset of carbon emissions cost	13
Rate of return and greenhouse gas emissions tax effect.....	18
Hydrogen demand curve parameters and technology breakthrough points	21
Hydrogen fuel demand parameters	21
Demand curve effect on hydrogen pathways	22
Feedstock and capital costs breakthrough points.....	28
Pathways succession sensitivity with respect to feedstock prices and capital costs.....	28
Natural gas feedstock and forecourt NG SMR capital costs variation	28
Biomass gasification capital costs and feedstock price variation.....	30
Electrolysis capital costs and electricity feedstock price variation	32
Prospects of forecourt electrolysis using surplus renewable energy.....	34
Concluding remarks.....	38
References	38
APPENDIX I. Hydrogen demand curve parameterization code	39

Figures and tables

Figure 1. Base case hydrogen pathway evolution scenario: hydrogen production	9
Figure 2. Base case hydrogen pathway evolution scenario: GHG emissions	9
Figure 3. Base case: GHG emissions and average production costs	10
Figure 4. Base case hydrogen pathway evolution scenario: cumulative capital costs	11
Figure 5. Base case hydrogen pathway evolution scenario: hydrogen costs at the pump	11
Figure 6. Base case: the number of production units and % employed	12
Figure 7. Cumulative GHG emissions from hydrogen production facilities: the GHG tax effect	13
Figure 8. Hydrogen pathways for GHG tax levels 10, 22, 26 and 80 \$/metric ton	14
Figure 9. Cost-optimal pathway evolution projection for GHG emissions tax at \$37/ton CO ₂ equivalent	15
Figure 10. GHG emissions tax at \$37/ton: Hydrogen costs evolution for a subset of pathways	16
Figure 11. Average hydrogen costs and GHG tax paid	16
Figure 12. Total capital costs of building hydrogen infrastructure: GHG tax effect	17
Figure 13. Rate of return and GHG tax effect on overall GHG emissions associated with H ₂ production	18
Figure 14. Hydrogen production with less expensive capital (IRR=7%)	19
Figure 15. Rate of return and GHG tax effect on H ₂ cost at the pump	19
Figure 16. Rate of return and GHG tax effect on overall capital costs	20
Figure 17. H ₂ demand curve parameterization. Line with crosses represents the demand curve	21
Figure 18. Original vs. parameterized demand curve	22
Figure 19. Cost-optimal pathways succession for parameterized and original H ₂ demand curves	22
Figure 20. Cost-optimal scenarios for various demand curves	23
Figure 21. Cumulative capital costs of building the hydrogen infrastructure for various demand curves	24
Figure 22. Production GHG emissions profiles for various demand curves	25
Figure 23. Hydrogen production scenarios for demand curves with varying maximum demand levels	26
Figure 24. Total capital costs of hydrogen infrastructure and production GHG emissions	27
Figure 25. Forecourt NG SMR capital costs effect on hydrogen pathways evolution	29
Figure 26. Cost-optimal hydrogen pathway evolution for increased forecourt SMR capital costs	29
Figure 27. Natural gas cost effect on hydrogen pathways evolution	30
Figure 28. Biomass feedstock cost effect on hydrogen pathways evolution	31
Figure 29. Cost-optimal hydrogen pathway evolution for decreased biomass feedstock costs	31
Figure 30. Biomass gasification capital costs effect on hydrogen pathways evolution	32
Figure 31. Cost-optimal hydrogen pathway evolution for decreased biomass gasification capital costs	32
Figure 32. Electricity cost effect on hydrogen pathways evolution	33
Figure 33. Cost-optimal hydrogen pathway evolution for decreased electricity price	34
Figure 34. Surplus renewable generation: Fraction of time occurring and usable fraction of surplus energy	35
Figure 35. Forecourt electrolysis capital costs effect with free surplus electricity	36
Figure 36. Hydrogen pathway evolution: free electricity and forecourt electrolyzer capital costs increased	37
Table 1 Key H2A default values as HyPro inputs	7
Table 2. Levelized hydrogen cost for several pathways in a generic H ₂ pathways evolution case	8
Table 3. Critical parameter values affecting hydrogen pathways scenario	37

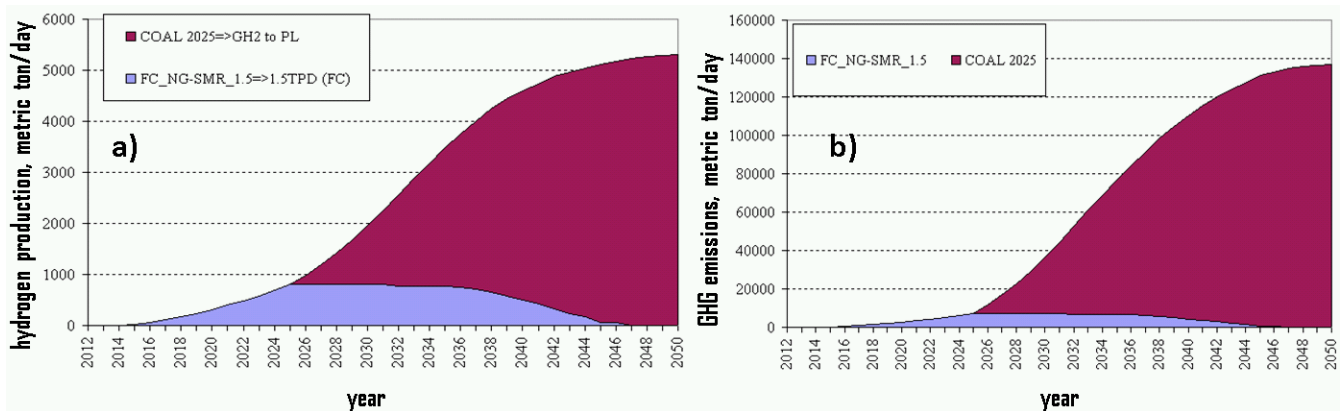
Summary

We are investigating a generic case of hydrogen production/delivery/dispensing pathway evolution in a large population city, assuming that hydrogen fuel cell electric vehicles (FCEV) will capture a major share of the vehicle market by the year 2050.¹ The range of questions that are considered includes i) what is the typical succession of hydrogen pathways that minimizes consumer cost? ii) what are the major factors that will likely influence this sequence?²

By combining infrastructure models from the DOE suite of hydrogen analysis tools, a high level approach (HyPro – MSM) is implemented that permits the evaluation of the potential evolution of a hydrogen infrastructure for FCEV. The HyPro – MSM framework provides estimates for generic analysis of key technological input effects and critical ‘tipping’ points which can potentially result in large changes in the hydrogen infrastructure buildout. Green-house gas emissions and hydrogen fuel cost at the pump are the focus of this report.

A typical set of HyPro-MSM outputs includes: i) a progression of H_2 cost-optimal³ pathways with the amount of hydrogen produced and delivered; ii) green-house gas (GHG) emissions associated with hydrogen production, cumulative and year-by-year; iii) capital costs for building the hydrogen infrastructure, cumulative and year-by-year. These data are analyzed over a wide range of a variety of input parameters.

The **base case scenario** uses default inputs from H_2 production and delivery models. The analysis shows the forecourt steam methane reforming (SMR) production option as the most cost-effective (by a large margin of $> \$1/kgH_2$) in the early years of hydrogen FCEV market development. This option is replaced by central coal gasification with pipeline delivery when the market matures and advanced technology options (both production and delivery) are available. The base case is associated with significant greenhouse gas emissions brought about by coal gasification.



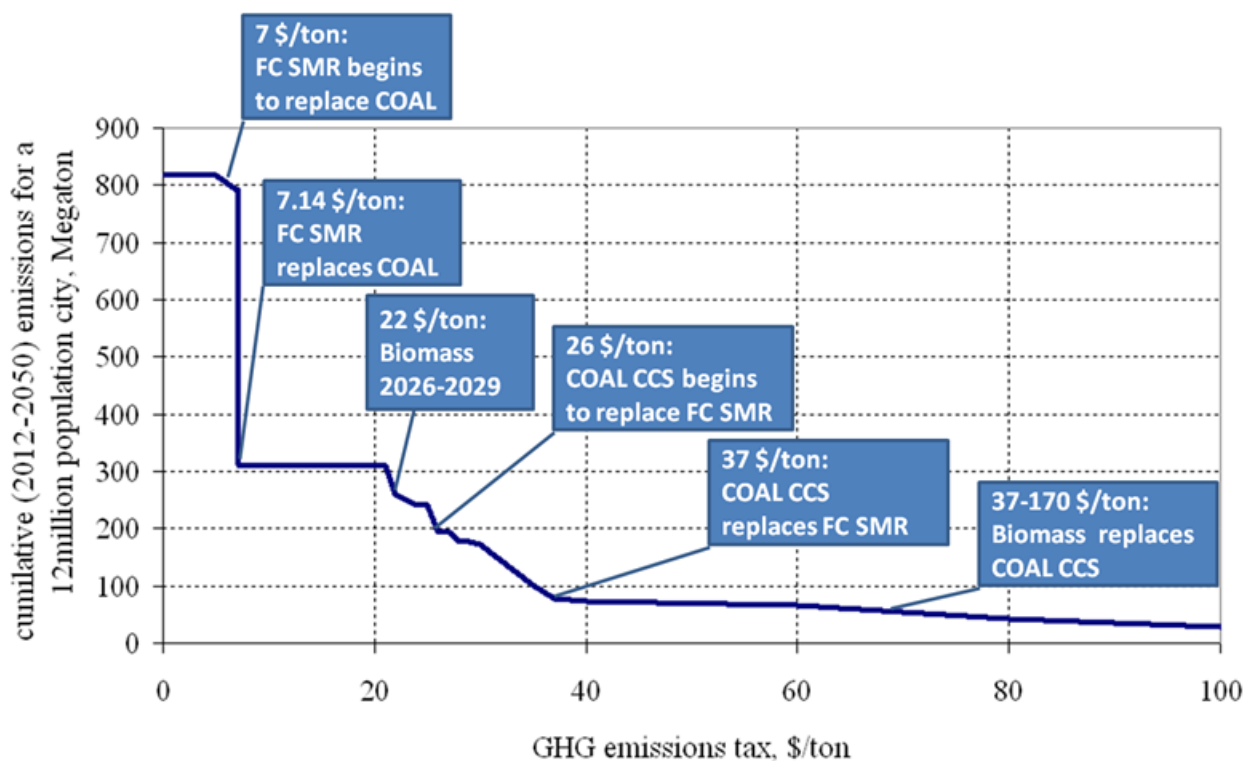
Base case scenario: a) hydrogen pathways evolution and b) GHG emissions associated with H_2 production.

¹ Fixed (i.e. pre-determined) hydrogen fuel demand curves are imposed externally to model hydrogen production/ delivery/ dispensing pathways. The demand dependence of production costs is accounted for in the form of learning curves.

² When a small change in parameter values induces a qualitative change in hydrogen pathways evolution, we call it a breakthrough point.

³ The model determines and schedules the least cost production option in a given year. There is no optimization over the time frame considered (2012-2050).

Potential effects of carbon emissions cost,⁴ a possible policy driver towards achieving cleaner hydrogen production technologies, are considered. Including a GHG emissions tax for hydrogen production into the HyPro-MSM framework affects the cost-optimal production options. Beginning with GHG tax values as low as \$7 / metric ton CO₂ equivalent, cleaner hydrogen production becomes economical and substantial GHG emissions reductions are possible in the long term (by 2050). Larger GHG tax values (above \$40/ton) result in further emissions decrease, although the effect is generally smaller as relatively clean production options are competing among themselves. The GHG tax effect on hydrogen cost is significant (up to \$1/kgH₂), but not prohibitive. More importantly, in the long term, most of the H₂ costs increase from the GHG tax goes towards funding cleaner hydrogen production rather than being collected as tax.⁵ The results do not show an increase in capital costs when shifting from coal gasification to less GHG-emitting technologies because less capital intensive options (e.g. biomass gasification) are employed along with more expensive production technologies such as coal gasification with carbon capture and sequestration (CCS).



Cumulative GHG emissions from hydrogen production facilities, years 2012 through 2050:
The effect of GHG emissions tax (dollars per metric ton).

Overall capital costs of building the hydrogen infrastructure, as expected, strongly depend on **the rate of return**. Lower IRR (7%) favors more expensive central production options and brings about early retirement of production facilities. High return rates (19%) not only eliminate early retirement, but also make the less capital intensive forecourt production option a heavy favorite.

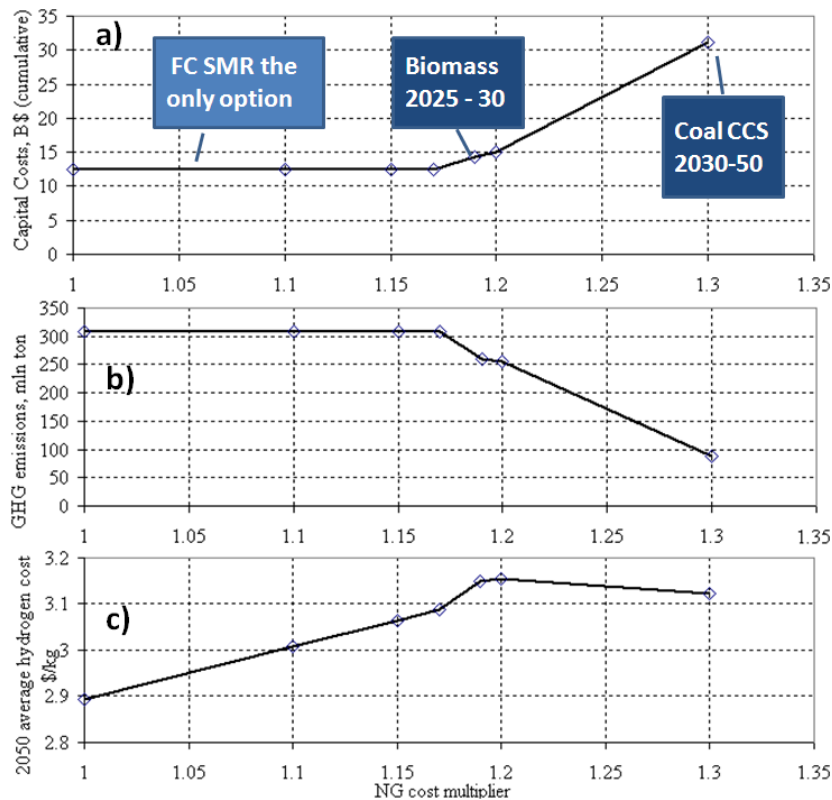
The broad range of city sizes, technology adoption rates and other circumstances will play a role in how the FCEV market develops. Here, we limit our inquiry to **changing the hydrogen demand evolution curve** and noting how these changes affect the expected technology evolution. The transition scenario is robust with respect to demand

⁴ Costs of carbon are discussed in this report in the form of a GHG emissions tax.

⁵ The cost of cleaner technologies plus the carbon tax is less than the cost of a 'dirtier' technology plus the carbon tax; cleaner technology is favored. The cost of production increases and the collected carbon tax decreases.

curve variations: relatively large changes in the demand curve parameters do not affect the succession of cost-optimal hydrogen pathways. The only exception is the maximum demand level; large demand levels favor central (coal) hydrogen production over forecourt SMR in the advanced stages of FCEV market development when the demand level is sufficiently large.

The analysis identified changes in **capital and feedstock costs** that would make clean hydrogen production technologies (biomass gasification, coal with CCS) cost competitive with the most cost effective option (forecourt SMR). Reaching a critical parameter value leads to considerable reduction of green-house gas emissions. With respect to NG feedstock prices, a 19% increase over the 2007 level will make biomass gasification cost-competitive. The same effect can be brought by a 30% or more decrease in biomass gasification capital costs or reducing biomass feedstock cost by half. Electrolysis from surplus wind electricity is competitive within a realistic range (27% to 35%) of capacity factor values.



Natural gas cost effect on hydrogen pathways evolution. a) cumulative capital costs (billion dollars), b) cumulative GHG emissions (million metric tons), c) average hydrogen cost at the pump (dollar per kilogram).⁶

While presented results provide a high-level overview on potential effects of most important (in our view) technological parameters, further analysis is required to assess geographic specificity and probe the effects of other numerous parameters that might trigger significant changes in hydrogen infrastructure buildout.

⁶ The capital costs (top subplot) and GHG emissions (middle) represent cumulative values for years 2012 through 2050. A slight increase in average hydrogen cost (bottom subplot) when the natural gas cost multiplier decreases from 1.3 to 1.2 is caused by early retirement of biomass gasification plants (built around year 2025 when the feedstock is relatively inexpensive but its price increases later).

Introduction

Transportation is a big part of the U.S. economy and is a major contributor of greenhouse gas (GHG) emissions. One of the realistic possibilities for mitigating the environmental impact of transportation is to replace traditional gasoline internal combustion engine vehicles with hydrogen-fueled fuel-cell electric vehicles (FCEV) [1]. The development of a suite of models and tools dedicated to hydrogen fuel cell electric vehicles [2] makes it possible to analyze various hydrogen production/delivery/dispensing pathways in terms of costs, GHG and other emissions, petroleum use (as a measure of dependence on foreign oil supply) and other parameters.

Macro-systems model (MSM)

When comparing hydrogen pathways, it is important to consistently propagate assumptions throughout the cross-cutting analysis of production, delivery and dispensing options. The macro-systems model (MSM) [3] has been developed to implement this goal. The MSM was designed as an overarching system for cross-cutting analysis and simulation capability to the U.S. Department of Energy's (DOE) Hydrogen Program. MSM was developed to accomplish the following specific objectives:

- To perform rapid, cross-cutting analysis in a single location by linking existing applicable models
- To improve consistency of technology representation (i.e., consistency between models)
- To allow for consistent use of hydrogen models without requiring all users to be experts in all models
- To support decisions regarding programmatic investments, focus of funding, and research milestones through analyses and sensitivity runs

HyPro: a hydrogen pathways progression analysis model

HyPro [4] is a MatLab-based computer model developed by Directed Technologies Inc. (DTI) under contract to the U.S. Department of Energy (DOE) for calculation of the expected "pump price" of hydrogen (i.e. the profited cost of hydrogen ready to be dispensed into a customer's vehicle at the dispensing station) for a variety of production/delivery/dispensing pathways in an area of uniform demand density over a span of years. By postulating the yearly hydrogen demand and calculating which supply infrastructure pathway is expected to provide the least expensive hydrogen in any given year, the model predicts how the infrastructure would be built out over time. This build-out prediction takes into consideration technology changes over time, underutilization of facilities in the early years of a station coming on line, potential stranded assets, feedstock costs differences, economies of scale in the production equipment, and "learning curve" capital cost reductions due to repetitious fabrication of multiple systems. The model allows for only one "winner" each year and all the pathways built that year will have the same combination of technologies. In reality, there is likely to be a diversity of opinion regarding demand level and price projections that will lead to more than one technology being built each year.

HyPro was linked with the MSM to provide updated consistency of HyPro input parameters with up-to-date versions of H2A Production [5] and HDSAM [6].

Analysis goals

We are investigating a generic case of hydrogen production/delivery/dispensing pathway evolution in a large population city, assuming that hydrogen fuel cell electric vehicles (FCEV) will capture a major share of the vehicle market by the year 2050. To compare various production and delivery possibilities, all central production facilities are assumed to be equally distanced from city boundaries. While HyPro has some flexibility in changing this assumption, more detailed models could be applied in dealing with specific geographic locations, as for example, SERA [7]. The range of questions that the MSM – HyPro tandem model is suitable to answer includes i)

what is the typical succession of hydrogen pathways that minimizes consumer cost? ii) what are the major factors that will likely influence this sequence?

Approach

In the course of this study, the HyPro model is used extensively in its integrated with MSM form. A typical set of HyPro-MSM outputs includes: i) a progression of H₂ cost-optimal pathways with the amount of hydrogen produced and delivered; ii) green-house gas emissions associated with hydrogen production, cumulative and year-by-year; iii) capital costs for building the hydrogen infrastructure, cumulative and year-by-year. These data are analyzed over a wide range of a variety of input parameters and our major findings are presented below.

Generic hydrogen pathways evolution scenario

As mentioned above, we are investigating a generic large city case (population ~12 million). By applying a hydrogen demand curve based on an extrapolation of optimistic projections within NAS 2004 report [1], an optimal progression of hydrogen pathways can be generated with the HyPro tool. This succession of production/delivery/dispensing technologies corresponds to the facility buildout that results in minimum hydrogen cost at the pump.

Model assumptions and inputs

Using the MSM, key HyPro inputs are updated to be consistent with latest HDSAM and H2A Production model versions. The key HyPro inputs derived from HDSAM and H2A Production models are listed in Table 1 below. Design capacity is given as the product between H2A default plant capacity and the yearly average capacity factor (90% for central and 85% for forecourt production options).

Default input values from HDSAM are used as inputs for terminal (gas and liquid H₂), delivery (liquid H₂ trucks and pipelines) and dispensing (1.5 ton/day) options. The advanced (i.e. after the year 2025) infrastructure options are adjusted to conform with Hydrogen Program goals as set in the DOE's Multi-Year Research, Development and Demonstration Plan [8], Table 3.2.2 Technical Targets for Hydrogen Delivery.

Central production facilities (upper part of the table) are assumed to be located at 60 miles distance from city gates, and a 40 mile by 40 mile city area is set as a HyPro input. GHG emissions data in the table are associated with hydrogen production; the central electrolysis options represent wind-powered electrolysis and bear no associated GHG emissions. Feedstock costs are used as given in the default feedstock cost tables, H2A Production models. The latter use EIA annual reports data [9]. Following current H2A assumptions, all projected costs are reported in 2005 U.S. dollars.

Hydrogen demand is the driving force behind the evolution of production, delivery and dispensing technologies, and the hydrogen demand curve is an important input to the model. We use the NAS projected national hydrogen demand profile [1], scaled down to suit the potential demand of the city. In our analysis, at maximal market penetration in the final year 2050, city hydrogen consumption levels off at $1.95 \cdot 10^9$ kg/year, which for a 12 million population city and 50% market penetration of FCEVs at 45 mi/GGE fuel efficiency results in approximately 14600 miles travel per vehicle per year. For this analysis, projected hydrogen production is equal to hydrogen demand in all years.

The model imposes an upper limit on distance between refueling stations (=6.95 miles). This parameter is used to determine the initial number of refueling stations within the city even though they may be initially severely underutilized. More stations are added as hydrogen demand surpasses dispensing capacity.⁷

⁷ In the model, refueling stations and production capacities are built to satisfy the next year demand.

Table 1. Key H2A default values as HyPro inputs.

Production or delivery technology	H2A model version	Design capacity ⁸ metric ton_H ₂ /yr	Depreciable capital, M\$	Feedstock efficiency GJ_H ₂ /GJ_feed ⁹	Feedstock cost ¹⁰ , \$/GJ	Utility NG GJ_H ₂ /GJ_NG	Utility electricity GJ_H ₂ /GJ_elec	Fixed O&M, M\$/yr	Other variable O&M Cents/kg_H ₂	Electricity byproduct efficiency GJ_H ₂ /GJ_elec	GHG emissions ¹¹ kg_CO ₂ /kg_H ₂
COAL 2005	2.1.1	103598	434.45	0.510	1.34	-	-	23.07	2.6	10.5	26.5
COAL 2025	2.1.1	80968	499.20	0.443	1.37	-	-	27.04	1.3	2.23	24.7
COAL CCS 2005	2.1.1	101071	690.13	0.553	1.34	-	19.4	28.65	2.7	-	1.98
COAL CCS 2025	2.1.1	80968	670.9	0.443	1.37	-	-	30.59	1.3	2.65	2.47
NG 2005	2.1.1	124628	180.49	0.729	6.07	-	58.5	6.92	1.7	-	9.28
NG 2025	2.1.1	124628	134.42	0.729	5.87	-	55.5	5.79	1.7	-	9.28
NG CCS 2005	2.1.1	124628	333.86	0.731	6.07	-	23.7	10.81	3.7	-	0.93
NG CCS 2025	2.1.1	124628	250.77	0.731	5.87	-	25.7	8.95	3.7	-	0.93
Biomass 2005	2.1.2	50908	154.39	0.479	1.27	19.3	34.0	10.39	0.3	-	0.44
Biomass 2025	2.1.2	50838	144.87	0.495	1.52	38.5	35.2	9.67	0.3	-	0.23
C Elys 2005	2.1.2	18517	110.41	0.625	14.9	-	-	5.41	2.3	-	0
C Elys 2025	2.1.1	18517	41.05	0.747	15.5	-	-	2.25	2.3	-	0
Nuclear HTE	2.1.1	268297	987.84	4.89 ¹²	4.78	-	1.01	55.94	-	-	0
GH ₂ terminal 2005	2.2	101071 ¹³	327.78	-	-	-	34.2	9.18	-	-	
GH ₂ terminal 2025	2.2	80968	246.85	-	-	-	33.4	2.38	-	-	
Pipeline	2.2	50838	0.28 ¹⁴	-	-	-	59.4	11.71	-	-	
Dispensing	2.2	465.4	1.48				10.3	0.286	-	-	
FC SMR 2005	2.1.2	465.4	1.139	0.73	6.07	-	30.1	.0750	0.4	-	9.26
FC SMR 2025	2.1.2	465.4	0.889	0.78	5.87	-	14.7	.0581	0.4	-	8.66
FC Elys 2005	2.1.3	465.4	2.738	0.623	14.9	-	-	0.184	4.1	-	43.4
FC Elys 2025	2.1.3	465.4	1.102	0.745	15.5	-	-	.0733	4.1	-	32.4
FC EtOH 2005	2.1.3	465.4	1.401	0.681	21.2	-	68.1	.0927	0.4	-	12.5
FC EtOH 2025	2.1.3	465.4	1.197	0.757	21.0	-	17.0	.0789	0.4	-	11.3

Where:

Coal= a coal gasification plant using technology of the year specified

CCS = Carbon Capture and Sequestration

NG= a Steam Methane Reforming plant

Biomass = biomass (wooden) gasification plant

C Elys = a central electrolysis plant

Nuclear HTE= high temperature electrolysis plant integrated with a nuclear power plant for heat and electricity supply

FC SMR= a distributed (i.e. forecourt) steam methane reforming plant

FC Elys= a distributed (i.e. forecourt) electrolysis plant

FC EtOH= a distributed (i.e. forecourt) ethanol reforming plant

⁸ Design capacity is given as the product between H2A default values for peak capacity and the yearly average capacity factor (90% for central and 85% for forecourt production options).

⁹ Energy related parameters (feedstock, utility and byproduct efficiency) in this table are based on lower heat values (LHV).

¹⁰ Feedstock costs in the table are given for years 2005 and 2025. The model uses EIA cost projections through 2050. The largest cost variation is projected for woody biomass (a four-fold increase from 2025 to 2050).

¹¹ GHG emission values are based on feedstock requirements and feedstock efficiency as given by H₂ production models and the associated emissions data as given by the GREET model. Where byproduct electricity is involved, the GHG emissions are assigned to hydrogen production. No credits (or penalties) are considered for producing less (or more) polluting electricity.

¹² Nuclear HTE uses heat (steam) and electricity with combined feedstock efficiency $0.83=(1/4.89+1/1.01)^{-1}$.

¹³ To match central production options, terminals are scaled up or down accordingly

¹⁴ Per mile pipeline

Hydrogen cost comprises production, delivery and dispensing costs. The breakdown of H₂ costs for the pathways that mirror production technologies listed in Table 1, is given in Table 2. All costs shown in those tables are for full utilization of the equipment over its life (in the model, equipment underutilization is allowed in which case stranded assets result in higher hydrogen costs). They also include assumptions that equipment production is sufficient to minimize production costs (i.e., economies of equipment production are met).

Table 2. Levelized hydrogen cost for several pathways in a generic H₂ pathways evolution case.

Pathway	production cost, \$/kg_H2	terminal cost, \$/kg_H2	delivery cost, \$/kg_H2	dispensing cost, \$/kg_H2	total cost, \$/kg_H2
COAL 2005, <i>via</i> liquid truck	2.24	2.72	0.31	1.36	6.63
COAL 2025, <i>via</i> pipeline	1.27	0.07	0.03	1.20	2.58
COAL CCS 2005, <i>via</i> liquid truck	3.33	2.71	0.31	1.36	7.72
COAL CCS 2025, <i>via</i> pipeline	1.73	0.08	0.03	1.20	3.05
NG 2005, <i>via</i> liquid truck	1.49	2.76	0.31	1.36	5.93
NG 2025, <i>via</i> pipeline	1.26	0.52	0.03	1.20	3.02
NG CCS 2005, <i>via</i> liquid truck	2.07	2.76	0.31	1.36	6.50
NG CCS 2025, <i>via</i> pipeline	1.51	0.52	0.03	1.20	3.26
Biomass 2005, <i>via</i> liquid truck	1.68	2.52	0.70	1.36	6.26
Biomass 2025, <i>via</i> pipeline	1.10	0.54	0.03	1.20	2.87
C Elys 2005, <i>via</i> liquid truck	4.59	2.62	0.31	1.36	8.89
C Elys 2025, <i>via</i> pipeline	3.17	0.62	0.03	1.20	5.03
Nuclear HTE, <i>via</i> pipeline	2.92	0.54	0.03	1.20	4.70
Existing H ₂ production, <i>via</i> liquid truck ¹⁵	2.00	2.62	0.31	1.36	6.58
FC SMR 2005	1.99			1.76	3.76
FC SMR 2025	1.52			1.20	2.72
FC Elys 2005	5.21			1.76	6.97
FC Elys 2025	3.12			1.20	4.33
FC EtOH 2005	4.98			1.76	6.75
FC EtOH 2025	4.13			1.20	5.33

Hydrogen pathways evolution: generic case

With the set of inputs described above, the model calculates the cost of each pathway for each year of the analysis to determine the optimal succession of pathways that results in the lowest cost of hydrogen at the pump while meeting the hydrogen demand curve (Figure 1). This analysis resulted in two production technologies and associated pathways that provide the least expensive hydrogen.¹⁶ In the early years (up to 2025) the forecourt SMR is the most cost efficient production technology with hydrogen being dispensed at forecourt stations with nominal capacities of 1.5 tonne/day. After 2025, coal gasification (without carbon

¹⁵ In the model, only the liquid H₂ truck option is available for delivery from the existing hydrogen production facilities.

¹⁶ The real-world production will probably include more diversity. Local/regional conditions including feedstock costs (electricity, biomass) and potential availability of existing infrastructure (eg, existing central production plants or pipelines) would likely influence a different mix than these two options.

capture and sequestration) with pipeline delivery becomes the lowest cost hydrogen supply pathway¹⁷ and growing demand is met by building coal with pipeline delivery infrastructure. Later, after 2036, as forecourt SMR stations retire, they are replaced by the more cost-efficient coal/pipeline option.

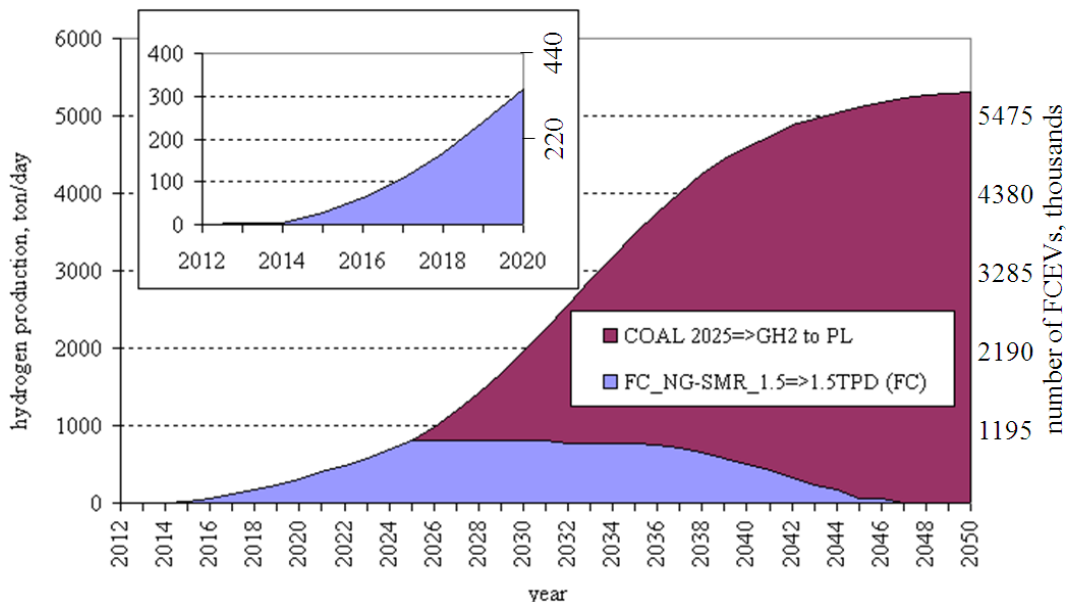


Figure 1. Hydrogen production (metric ton per day) for the base case hydrogen pathway evolution scenario. The axis on the right shows the corresponding number of fuel cell vehicles assuming 45 mi/GGE and 14600 mi/year for an average vehicle. The insert shows the assumed early-years H₂ demand growth.

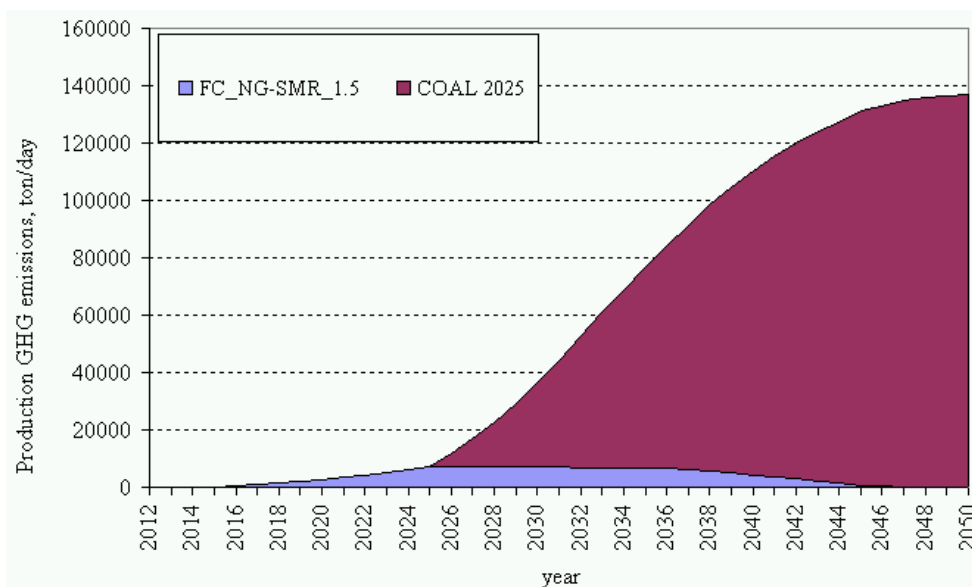


Figure 2. GHG emissions (metric ton CO₂ equivalent per day) for the base case pathway evolution scenario.

The output from HyPro also provides data on the GHG emissions associated with each production pathway (Figure 2). As expected, the GHG graph follows the general contours set by the Figure 1 data, with correction for different scales and adjustment for the significantly higher GHG emissions from coal feedstock over that of natural gas (on a per kg H₂ basis, see also Table 1). In this scenario, as the natural gas feedstock is gradually

¹⁷ We assume that pipeline delivery is only available in 2025 or later. Before 2025, only (more expensive) truck delivery options are available.

replaced by coal after year 2025, average GHG emissions associated with producing 1 kg of hydrogen are increasing (Figure 3a). The hydrogen cost decrease (Figure 3b) in the early years (2010 to 2015) occurs because the production facilities are more fully employed. Lower H₂ cost in 2025 becomes possible due to hydrogen production by coal gasification. It should be noted that the hydrogen price evolution is primarily driven by feedstock price values, also shown (for years 2005 and 2025) in Table 1.

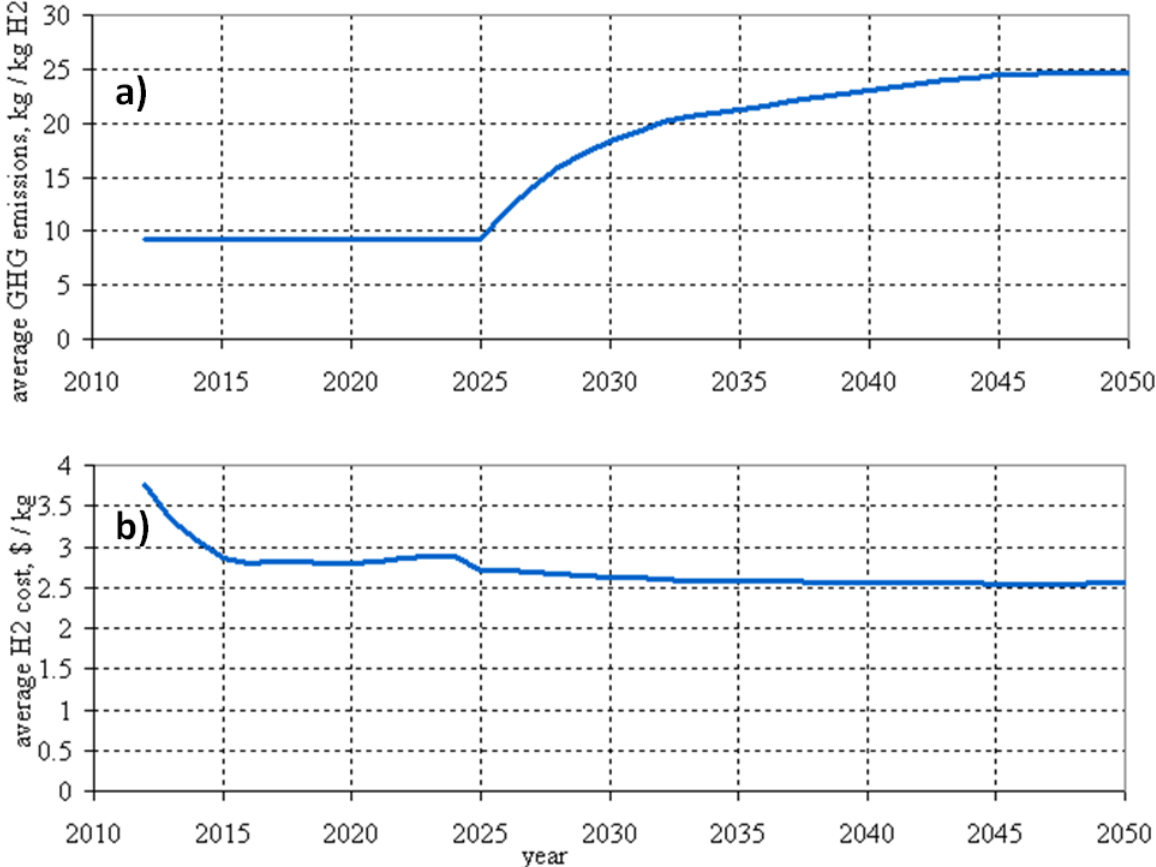


Figure 3. Base case: a) GHG emissions (in terms of weight CO₂ equivalent) associated with producing 1 kg hydrogen and b) average production costs

Capital costs incurred to build the hydrogen infrastructure are also an important aspect of the pathway evolution scenario and are shown in Figure 4. In the early stages of FCEV market expansion before 2025, hydrogen production and dispensing account for all the capital expenses (since all hydrogen is supplied by forecourt SMR units that do not incur delivery costs). After 2025, when central production facilities begin to dominate, hydrogen terminals and delivery account for a 30% share of expenses. By the year 2050, production facilities still account for the largest portion of capital costs, but hydrogen terminals, pipelines and dispensing account for more than half of the cumulative ‘price tag’.

Naturally, hydrogen production costs are among the important features that are determined by the model. The following graph (Figure 5) displays hydrogen costs for several pathways analyzed by the model (there are more than 50 pathways and it is not practical to show H₂ costs for all of them). Hydrogen pipelines are only allowed

starting in 2025: hence many new pathways spring into being in that year. Step changes in hydrogen price in 2025 are induced by the assumed step changes in technology (production, terminals, delivery and dispensing).¹⁸

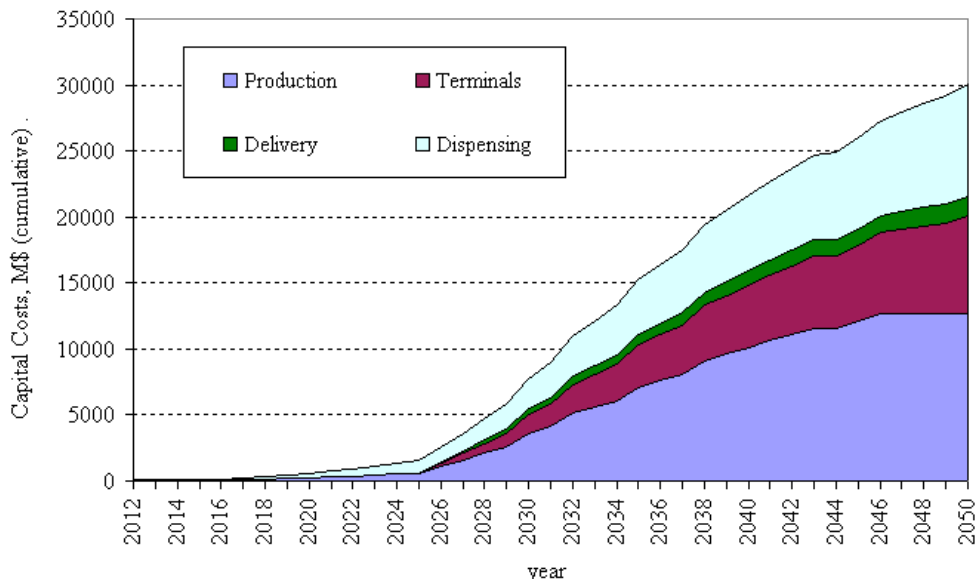


Figure 4. Base case hydrogen pathway evolution scenario: Cumulative capital costs of building the hydrogen infrastructure, by year

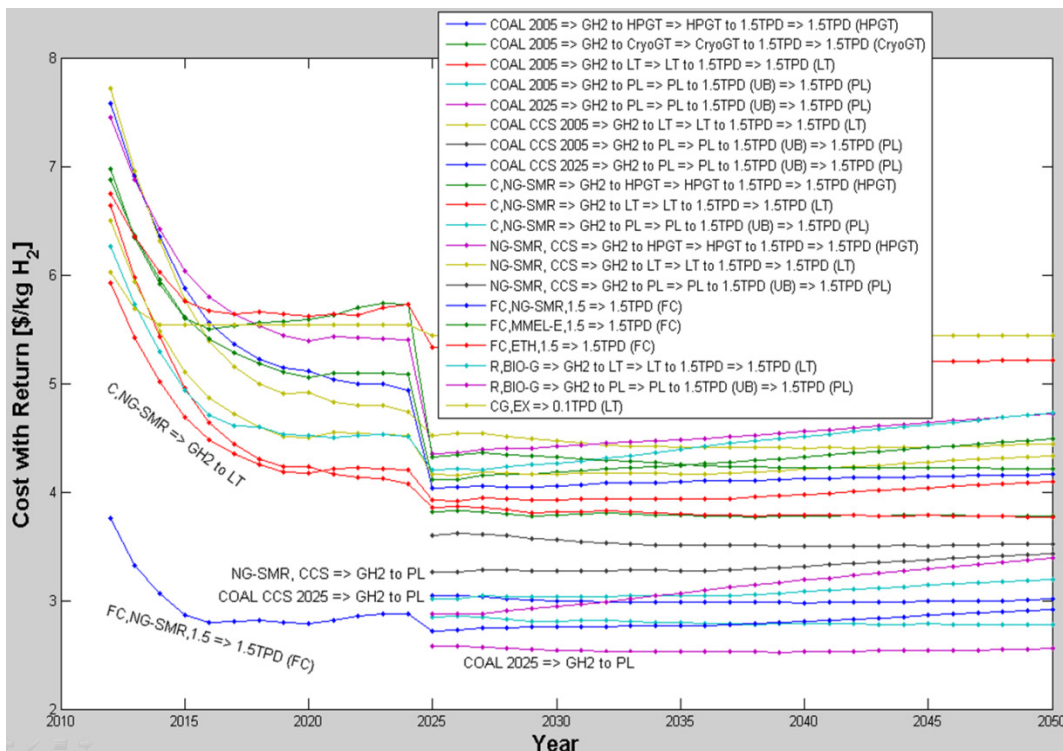


Figure 5. Base case hydrogen pathway evolution scenario: Hydrogen (at the pump) costs for a subset of pathways at each startup year

¹⁸ Figure 5 represents the dynamics of marginal H₂ costs (for the newly built capacities only). This is why some curves on the figure show sharp changes in 2025 when new less expensive technologies become available in the model. The dynamics of average H₂ cost is significantly smoother.

In the early years, when hydrogen demand is low and production and dispensing facilities are engaged well below their capacity limits (see also Figure 6), hydrogen production costs are significantly higher. For forecourt (smaller scale) production options (e.g. FC NG SMR) this trend ends by the year 2016 and further variations in H₂ costs are induced mostly by changes in the projected feedstock prices and technology improvements (in 2025). Central production (e.g. C NG SMR) requires higher demand levels (that are reached in ~2020) to saturate its capacity. The forecourt SMR production is the most cost efficient technology by a large margin until the year 2025, when pipeline delivery (the least expensive delivery option when highly utilized) becomes available and makes central production options competitive. The average production cost of hydrogen (Figure 3b) reflects these trends.

The underutilization of production capacities (Figure 6) for distributed production (FC SMR) occurs early in conditions of low demand due to a minimum number of stations defined so that a maximum distance requirement between them is met. All stations are fully utilized by 2016, due to sharp demand growth, and additional stations are needed in following years. When the market is saturated (years 2045-2050), existing coal production capacity warrants early retirement of forecourt production units.¹⁹

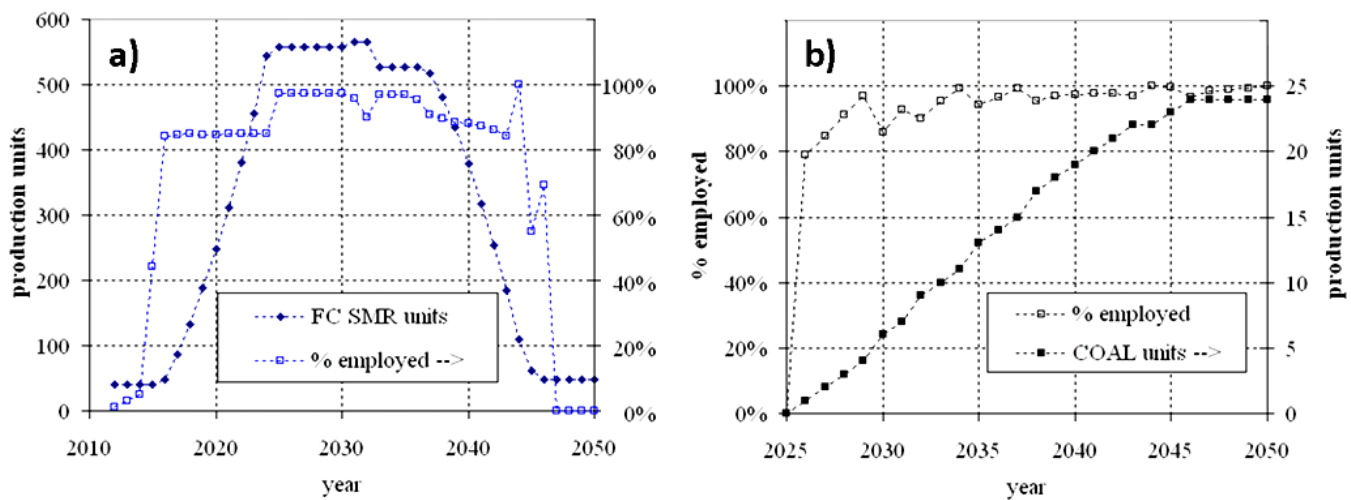


Figure 6. Base case hydrogen pathway evolution scenario:
the number of production units and % employed for a) FC SMR and b) coal.

The base case scenario was created by using H2A Production and HDSAM defaults. It shows the forecourt SMR production option as the most cost-effective (by a large margin of > \$1/kgH₂) in the early years of hydrogen FCEV market development. This option is replaced by central coal gasification with pipeline delivery when the market matures and advanced technology options (both production and delivery) are available. The base case is associated with a significant greenhouse gas emissions level brought about by coal gasification.

¹⁹ The costs of stranded (due do early retirement) assets are included in the hydrogen cost; the capital costs of facilities that retire early are recovered in the model.

Greenhouse gas emissions mitigation

The generic base case is GHG emission agnostic in that it simply reflects the current state of affairs where GHG emissions are not factored into the economic calculations or pathway selection metric. While consumers and policy makers can make emissions count in a variety of ways, we expect the result to reflect as a penalty for higher GHG emitting technologies or a stimulus for lower GHG emitting options or both. In the present study, we differentiate hydrogen production options via the cost of carbon-containing emissions. Below, we consider potential effects induced by various levels of GHG emissions tax as a possible policy driver towards achieving cleaner hydrogen production technologies.

Base case hydrogen pathways with the onset of carbon emissions cost

The GHG emissions tax, in the form that it is considered within the MSM-HyPro framework, penalizes GHG emissions (in terms of CO₂ equivalents) at the hydrogen production stage. For all feedstocks the upstream emissions are included and assessed as part of the GHG tax cost. The right column in Table 1 provides a basis for applying the hydrogen production GHG tax. Production technologies with the highest GHG emissions per kg H₂ will be penalized the most. At any rate, the GHG tax is ultimately reflected in the hydrogen cost at the pump. Here, we are not specifically interested in the GHG tax fiscal (i.e. to raise revenue) effect; rather, the goal is to stimulate the development of cleaner hydrogen production options. By imposing different tax rates as HyPro model inputs, we look for critical tax levels that trigger changes in pathway evolution scenarios.

It is convenient to begin the discussion of the GHG emissions tax effect by analyzing the plot that summarizes GHG emissions reduction as a function of GHG emissions tax level (Figure 7).

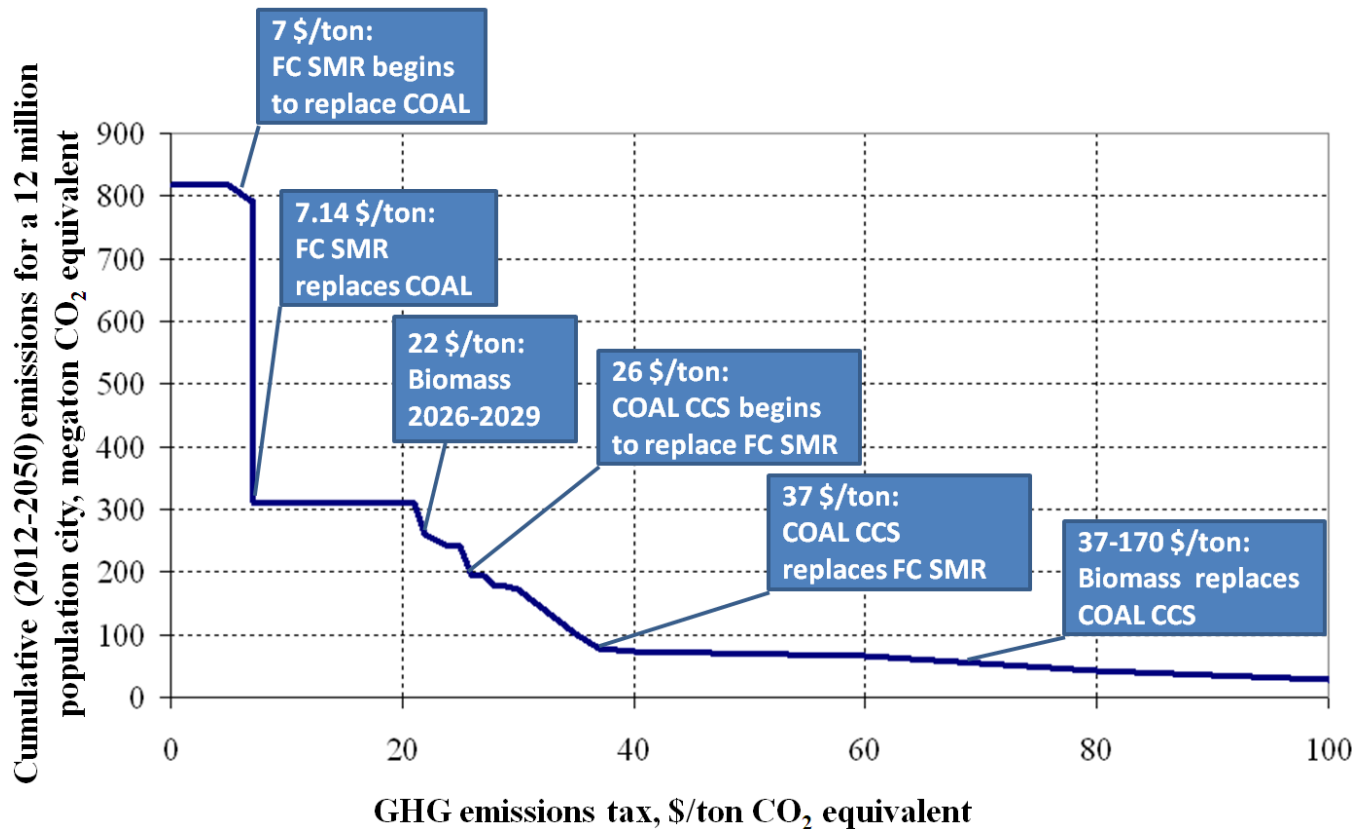


Figure 7. Cumulative GHG emissions from hydrogen production facilities, years 2012 through 2050: The effect of GHG emissions tax (dollars per metric ton CO₂ equivalent).

Small GHG emissions tax levels do not affect the technology mix or the GHG emissions. Then, at fairly low tax levels (7-7.14 \$/metric ton CO₂ equivalent), FC SMR (forecourt steam methane reforming) becomes more economical than coal gasification and results in a large (62%) reduction in the overall amount of greenhouse gas emissions. Further increase in the GHG tax level (up to 21\$/metric ton) does not induce any technology changes: between 7.14 and 21 \$/ton the cost optimal scenario involves only forecourt SMR hydrogen production for any year under consideration (2012-2050, Figure 8a). In the tax level range between 21 and 37 \$/ton, several changes occur gradually in an overlapping fashion.

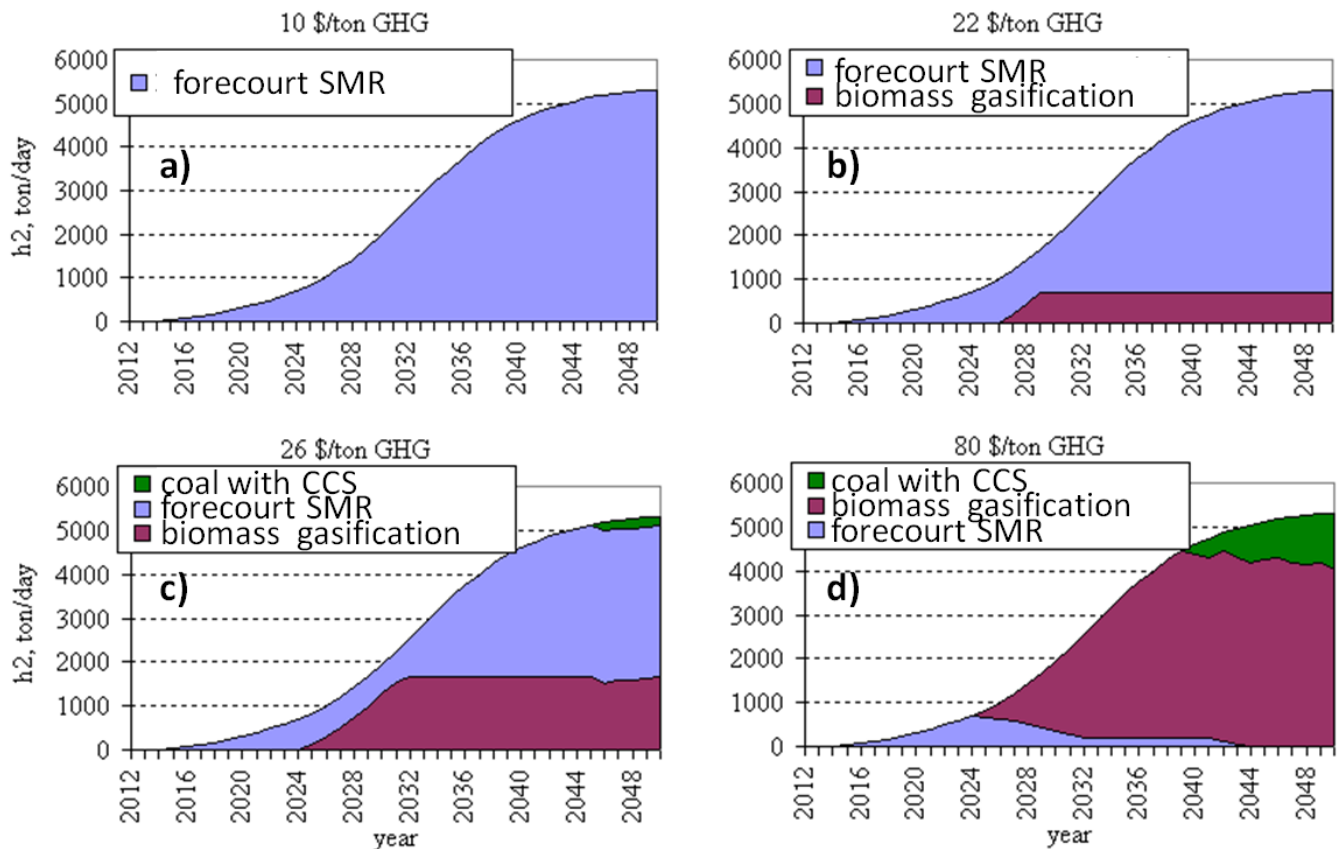


Figure 8. Hydrogen pathways for GHG tax level a) 10, b) 22, c) 26, d) 80 \$/metric ton CO₂ equivalent

Biomass gasification becomes competitive (Figure 8b) for several years at \$22/ton tax level. (Biomass feedstock projected price is gradually increasing so there is no sharp takeover as in the COAL – FC SMR case at ~\$7/ton tax). Between 26 and 37 \$/ton tax levels (Figure 8c) coal gasification with carbon capture and sequestration (COAL CCS) replaces forecourt SMR as the preferred advanced technology option (for years 2027-2050). The pathway evolution scenario at \$37/ton GHG emissions tax level is presented in more detail on Figure 9.

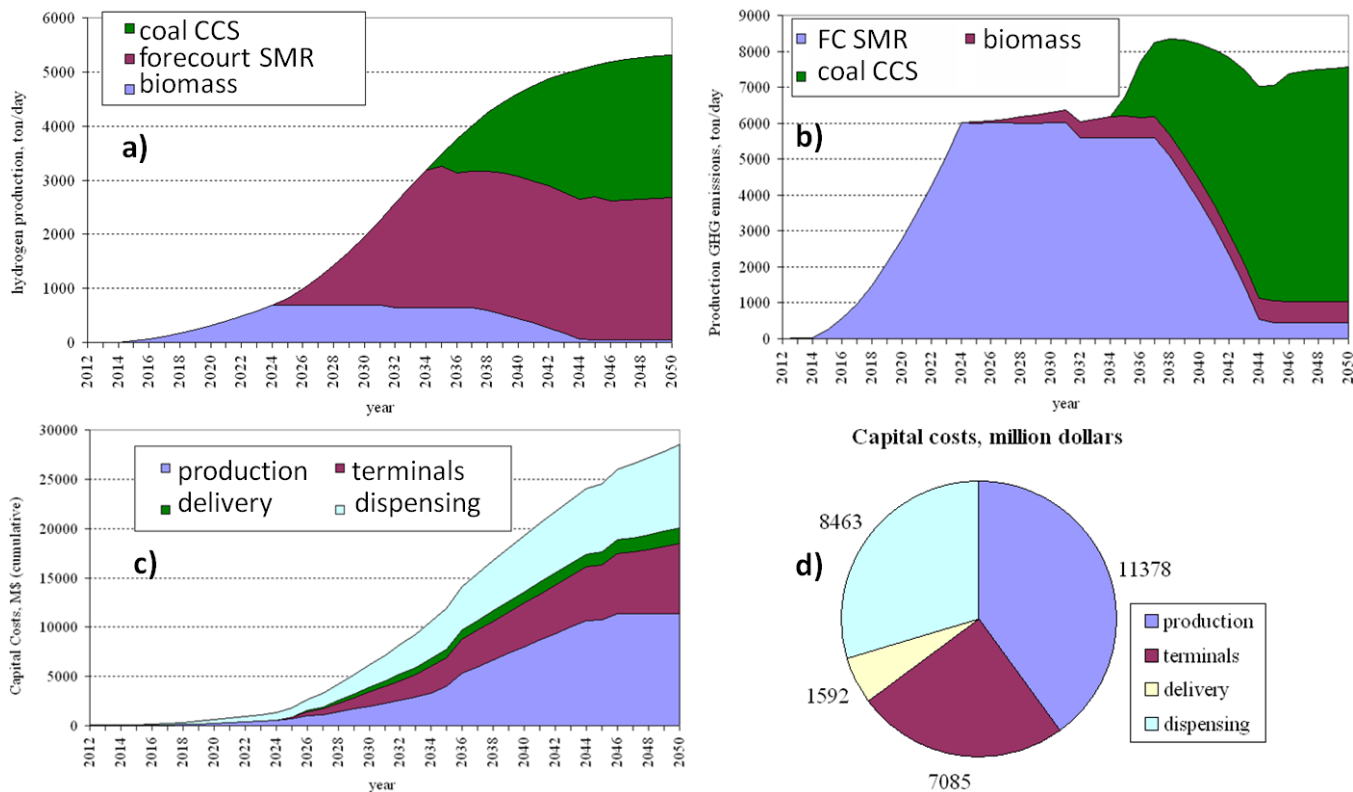


Figure 9. Cost-optimal pathway evolution projection for GHG emissions tax at \$37/ton CO₂ equivalent:
a) Hydrogen production dynamics (by pathway); b) GHG emissions;
c) cumulative capital costs and d) total capital costs by the year 2050.

At a GHG emissions tax level of 37 \$/metric ton, clean hydrogen production technologies dominate the advanced stages of H₂ FCEV market. Forecourt SMR production facilities are not built after 2025, the demand increase is satisfied by biomass gasification and, after 2034, both growth in hydrogen demand and retiring FC SMR units are compensated by coal gasification with carbon capture and sequestration. The GHG emissions level is significantly lower than the emissions in the zero-GHG tax case (Figure 2). In 2050, COAL CCS supplies approximately half the H₂ demand and Biomass gasification supplies approximately one-third the H₂ demand.

The cost of building the infrastructure (for the entire 12 million person city over 38 years) is slightly below the \$30 billion mark for the zero-GHG tax case (Figure 4) and decreases with the onset of GHG tax (Figure 9) because less capital intensive biomass gasification is employed along with more expensive coal gasification with carbon capture and sequestration. Hydrogen fuel costs are determined by the interplay of three curves (FC SMR, Biomass, and COAL CCS) on the hydrogen pathways costs map (Figure 10). As mentioned above, with time the biomass option loses its competitiveness because of the projected feedstock price growth.

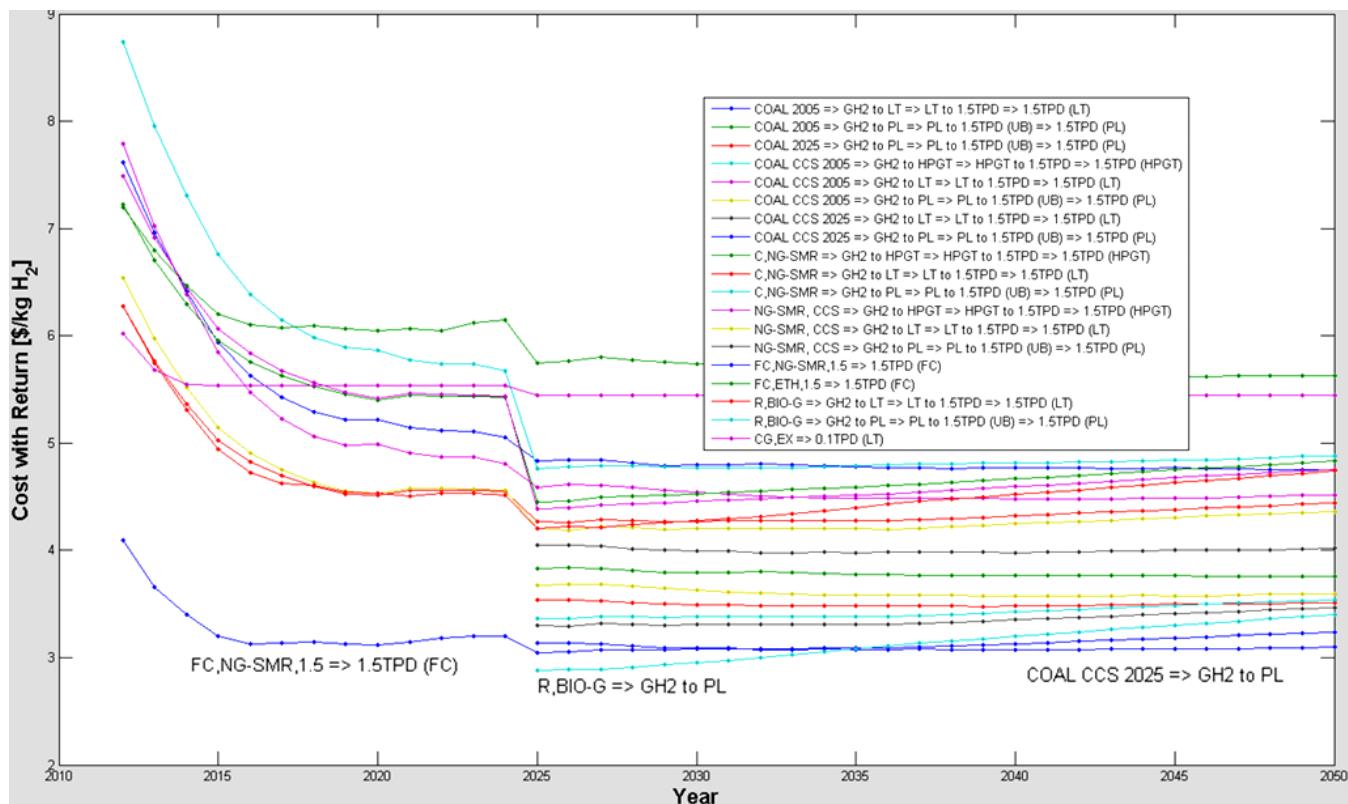


Figure 10. GHG emissions tax at \$37/ton: Hydrogen costs evolution for a subset of pathways.

In Figure 11, we plot both the average H₂ cost and the amount paid as GHG tax, for years 2025 and 2050.

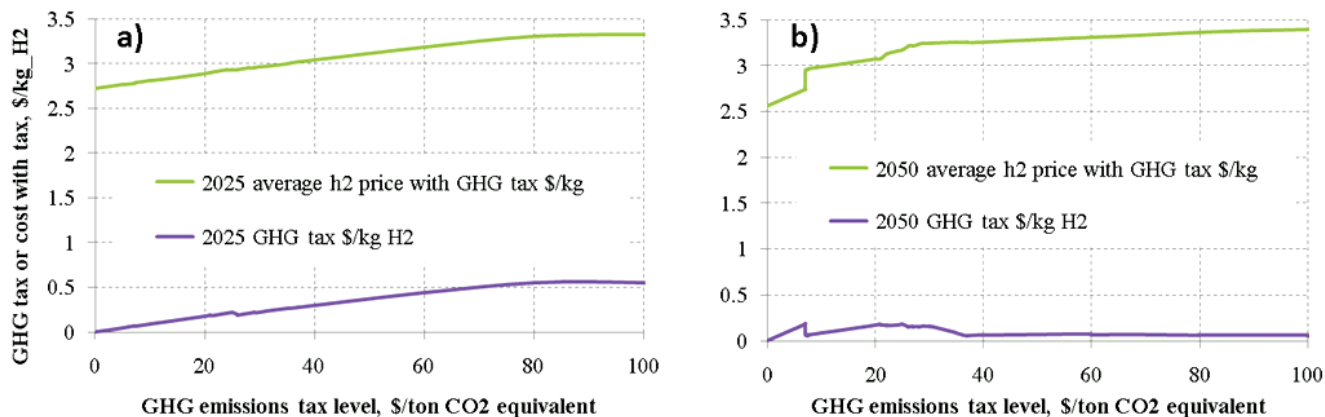


Figure 11. Average hydrogen costs and GHG tax paid in a) 2025 and b) 2050.

The early-stage technology (before 2025) is not affected by increasing GHG tax level and all of the hydrogen cost increase is paid by the consumer as a GHG emissions tax;²⁰ the tax has mostly a fiscal revenue effect. The mature H₂ market (2050) is significantly impacted by the GHG tax, and the amount of GHG tax collected is much smaller than the H₂ cost increase. In 2050 the consumer pays mostly for the deployment of cleaner technology; the tax has mostly a technological effect.

²⁰ Presumably, the hydrogen cost increase can be partially avoided by imposing a cap and trade policy rather than a GHG emissions tax, with the intent of differentiating production technologies based on associated GHG emissions. The implications of ‘cap and trade’ deserve a separate study and are not included in this report.

Irregularities observed on the hydrogen cost and GHG tax curves for the year 2050 (Figure 11b) are inflicted by technology breakthrough points that are described above in connection with Figures 7 and 8. The same technology break-even points reflect on overall capital costs (Figure 12).

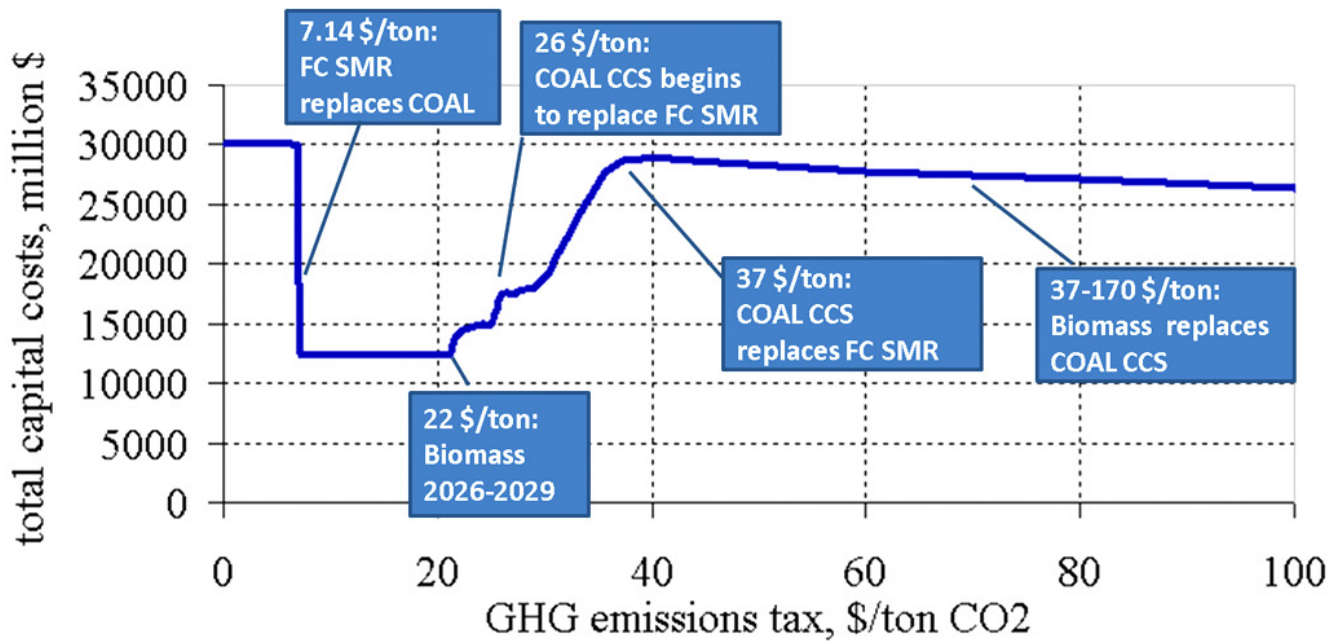


Figure 12. Total capital costs of building hydrogen infrastructure: GHG tax effect.²¹

The variation of capital costs with the onset of GHG tax is largely affected by the differences in capital costs for FC SMR, COAL, COAL CCS and Biomass production technologies. Lower capital costs for FC SMR cause a large decrease on the graph when the GHG tax exceeds \$7/ton and forecourt natural gas reforming replaces coal gasification for years 2025 through 2050. Conversely, further increase in GHG tax level leads to higher capital costs because FC SMR is replaced by cleaner and more capital intensive production technologies (Biomass and COAL CCS).

*Including a greenhouse gas emissions tax for hydrogen production into projected pathways evolution analysis within HyPro-MSM network shows promising results in terms of the tax effect on cost-optimal production options. Beginning with GHG tax values as low as \$7 / metric ton CO₂ equivalent, cleaner hydrogen production becomes economical and substantial GHG emissions reductions are possible in the long term (by 2050). Larger GHG tax values (above \$40/ton) result in further emissions decrease, although the effect is generally smaller as relatively clean production options are competing among themselves. The GHG tax effect on hydrogen cost is significant (up to \$1/kgH₂), but not prohibitive. More importantly, **in the long term, most of the H₂ costs increase induced by the GHG tax goes towards funding cleaner hydrogen production rather than being collected as tax. The results do not show an increase in capital costs when shifting towards less GHG-emitting technologies because biomass gasification (which requires less capital costs) becomes competitive along with more capital intensive coal with CCS option.***

²¹ The zero-GHG emissions tax case is discussed above in the “Hydrogen pathways evolution: generic case” section. This case favors coal gasification production option. The less carbon-emitting forecourt SMR option is a close competitor (Figure 5) and a relatively small GHG emissions tax level (\$7/ton) makes forecourt SMR the cost-optimal choice.

Rate of return and greenhouse gas emissions tax effect

Capital investment requirements are an important factor that ultimately reflects on hydrogen cost at the pump. While HyPro allows exploring the capital cost sensitivities of individual production options, the rate of return is a parameter that affects the relative importance of capital costs of all technology components. Below, we apply this *en masse* approach to investigate what technology breakthrough points are most sensitive to capital cost values.

The default real internal rate of return after tax (IRR) for H2A Production and HDSAM models is 10% and this value was applied when obtaining results described above. Here, two other IRR values are considered. IRR of 7% would correspond to cases with significant portion of capital costs being covered by government guaranteed loans. The 19% IRR value simply corresponds to double investment value in four years²². As expected, these two IRR values lead to different GHG tax trigger points for controlling the cost-efficient sequence of hydrogen fuel production options (Figure 13).

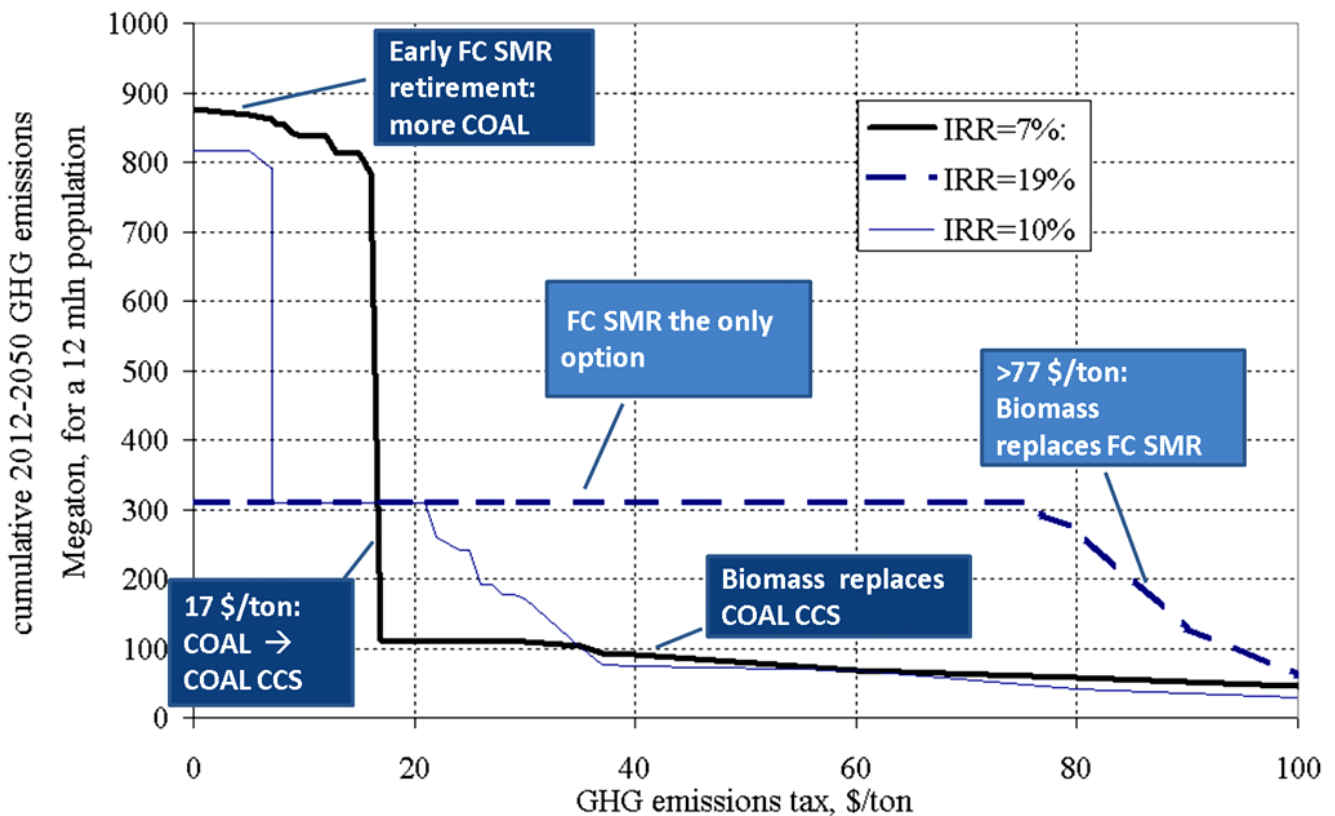


Figure 13. Rate of return and GHG tax effect on overall GHG emissions associated with H₂ production.

When lower return rates are allowed (i.e. less expensive capital is available), existing FC SMR units are retired early and replaced by central coal gasification facilities (Figure 14a vs. Figure 1 and 14b vs. Figure 9a). For low GHG tax levels, this incurs higher greenhouse gas emissions than in the generic base case (Figure 7). The low IRR value (7%) allows for early retirement of production facilities (both zero-GHG tax and \$37/ton tax cases show this effect).

²² At this annual rate of return the investment doubles over the course of four years: $(1.19^4)^2 = 2.005$.

The high-level IRR (i.e. more expensive capital) leads to less diversity in the cost-optimal technologies. Only the least capital intensive (FC SMR) and the most green-house gas efficient (Biomass) options are ever selected throughout the entire range of years and GHG tax levels.

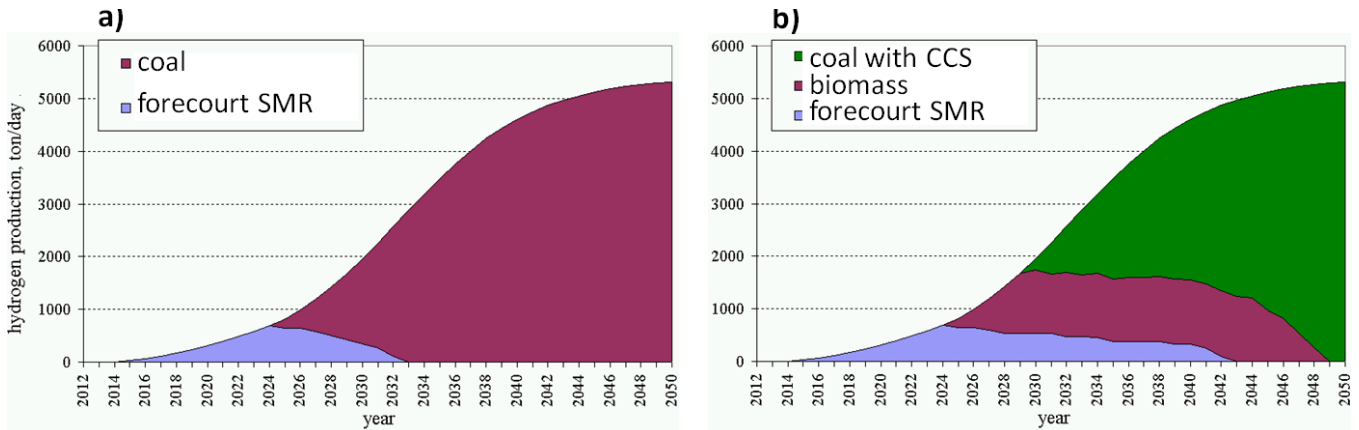


Figure 14. Hydrogen production with less expensive capital (IRR=7%): a) no GHG tax and b) \$37/ton GHG tax. Both cases exhibit early retirement of production facilities (a: FC SMR and b: Biomass).

Lower IRR case (7%, Figure 15a) demonstrates different behavior from the moderate IRR (10%, Figure 11b). Sharp technological changes do not lead to price hikes (Figure 15a at ~\$17/ton) at lower rates of return. Moderate return rate (10%, Figure 11b at ~ \$7/ton), however, shows a H₂ cost hike²³. For high IRR values (19%) the GHG tax is inefficient in triggering a technology shift towards cleaner production options: GHG emissions reductions are achieved only at tax levels approaching \$100/ton CO₂.

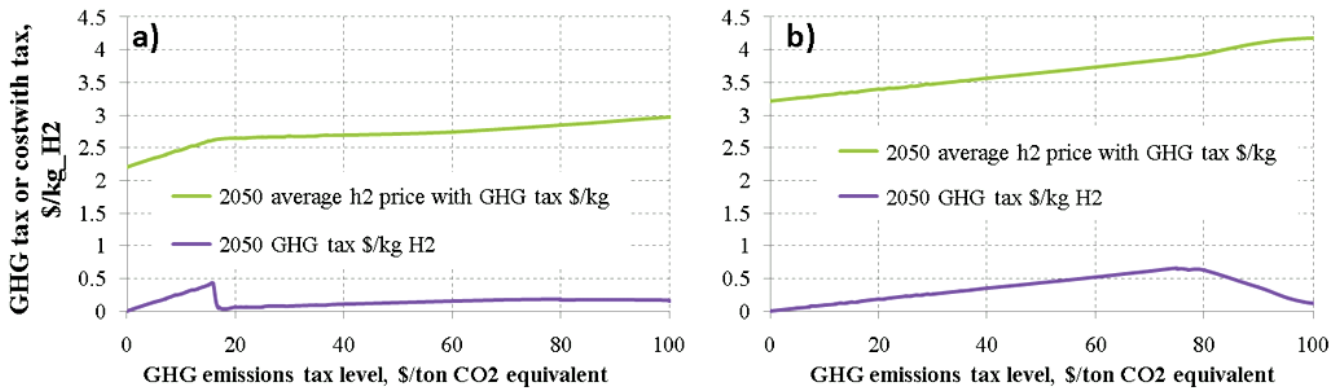


Figure 15. Rate of return and GHG tax effect on H₂ cost at the pump. a) IRR=7%; b) IRR=19%

²³ For higher return rate values, it is too expensive to early retire existing (FC SMR) units, and forecourt production can better accommodate the smooth-growing demand than the large-scale central production plants; for these reasons the model keeps building slightly sub-optimal facilities which manifests itself as a sharp cost increase on the cost vs. GHG tax plot.

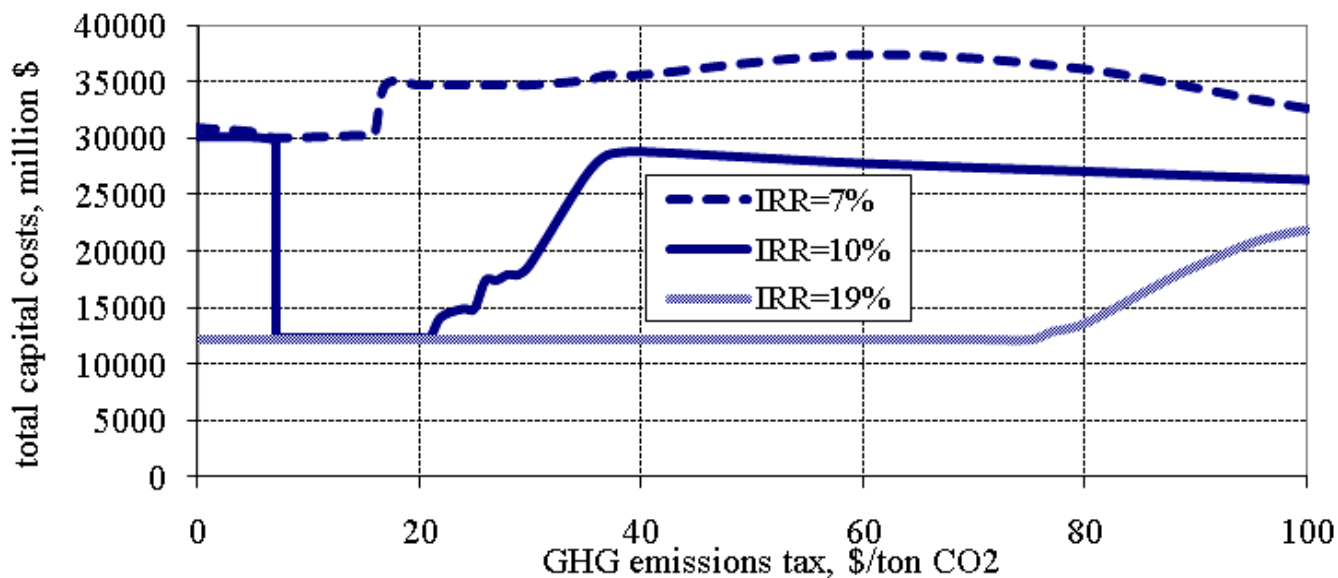


Figure 16. Rate of return and GHG tax effect on overall capital costs

Overall capital costs of building the hydrogen infrastructure, as expected, strongly depend on the rate of return (Figure 16). Lower IRR (7%) favors more expensive central production options and tends to allow early retirement of production facilities.²⁴ High return rates (19%) not only disallow early retirement, but also make forecourt production a heavy favorite.

All further results are given for the default 10% value of the rate of return.

²⁴ The wide maximum near \$60/ton tax results from retirement of biomass units in favor of newly built COAL CCS.

Hydrogen demand curve parameters and technology breakthrough points

At this time, one can imagine a variety of ways the hydrogen fuel demand will evolve, and none of them with a high level of certainty. There is a broad range of city sizes (reflecting in the maximum demand level), technology adoption pace (resulting in demand growth rates) and other circumstances that will play a role in how the FCEV market will develop. Here, we limit our inquiry to changing the hydrogen demand evolution curve and noting how these changes affect the observed technology breakthrough point.

Hydrogen fuel demand parameters

First, we approximate the generic demand curve based on the NAS recommendations [1] with an analytic expression that has a manageable number of parameters. Then we compare HyPro results that use the constructed parameterized curve with the generic base case results. Next, the parameter values are varied to examine their effect on hydrogen pathways breakthrough points.

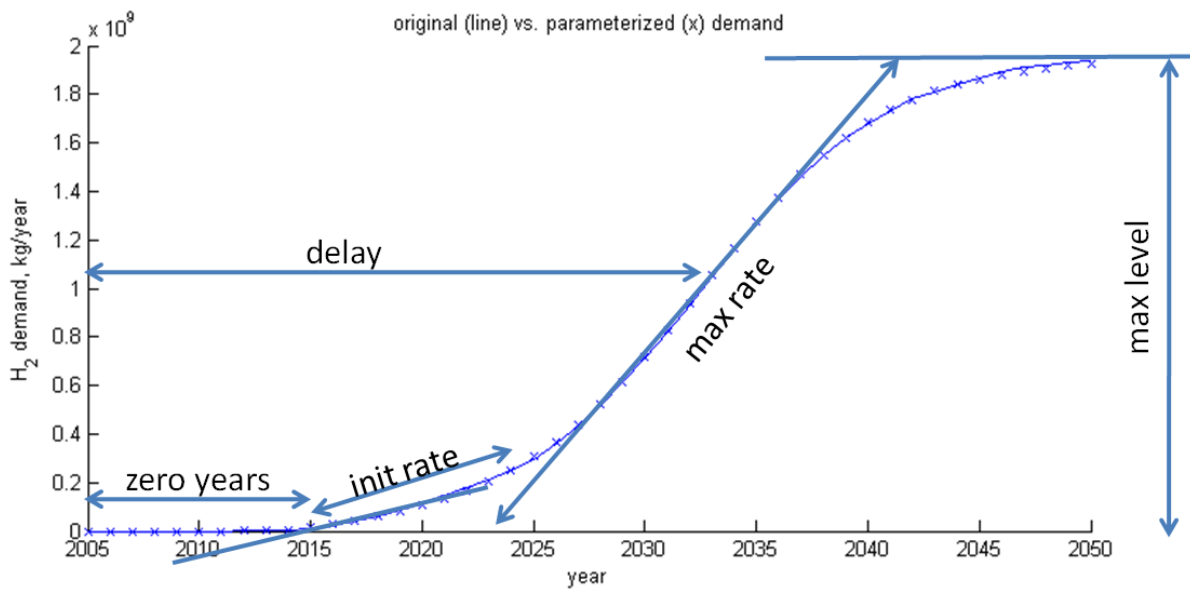


Figure 17. H₂ demand curve parameterization. Line with crosses represents the demand curve.

The mathematical expression involving the parameters described qualitatively in Figure 17 is rather complicated. We present the matlab version of the computer routine used for calculating the parameterized demand curve in the Appendix I. The max rate of annual H₂ demand growth is defined as the number of years needed to reach the maximum level (i.e. full H₂ FCEV market penetration) at this maximum growth rate: thus 12.1% of full demand per year corresponds to approximately 8 years. Similarly, the initial demand growth rate of 0.35% of full demand per year means that at this pace it would take approximately 300 years to saturate the market. 'Zero years' specifies the number of years (starting in 2005) before H₂ demand begins to grow. And the time lag (marked as 'delay' on Figure 17) gives the period of time until the maximum demand growth rate is initiated.

As shown in Figure 18, the correlation between the original H₂ demand curve and the parameterized curve is very good. Correspondingly, the resulting HyPro generated cost-optimal pathways succession (Figure 19a) for the parameterization is very close to that generated based on the original demand curve (Figure 19b).

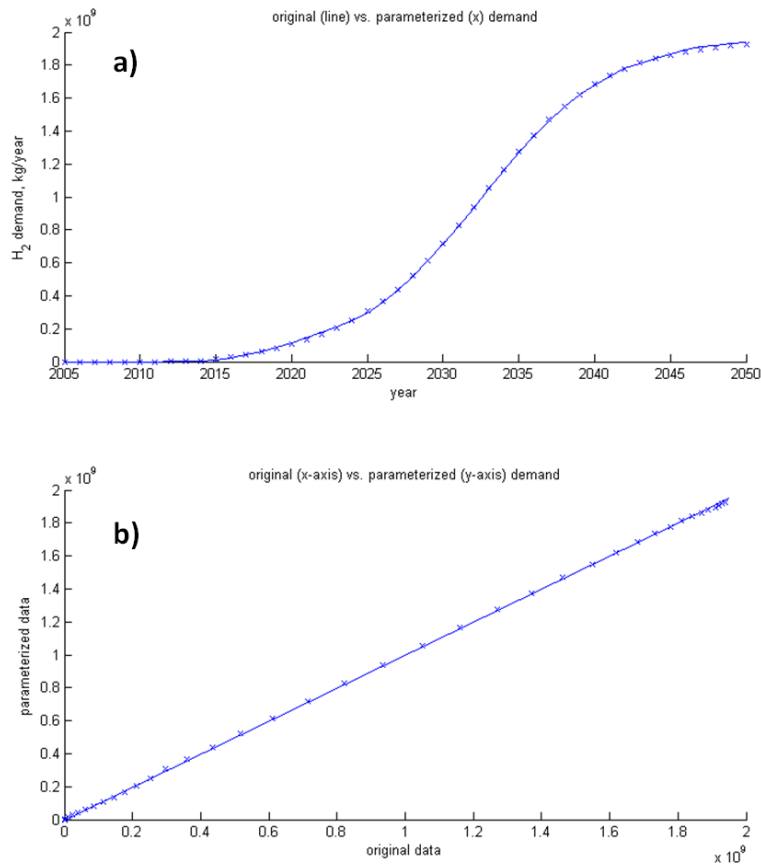


Figure 18. a) Original (line) vs. parameterized (crosses) demand curve; b) crosses: original vs. parameterized demand curve, the line represents the exact equality between the two.

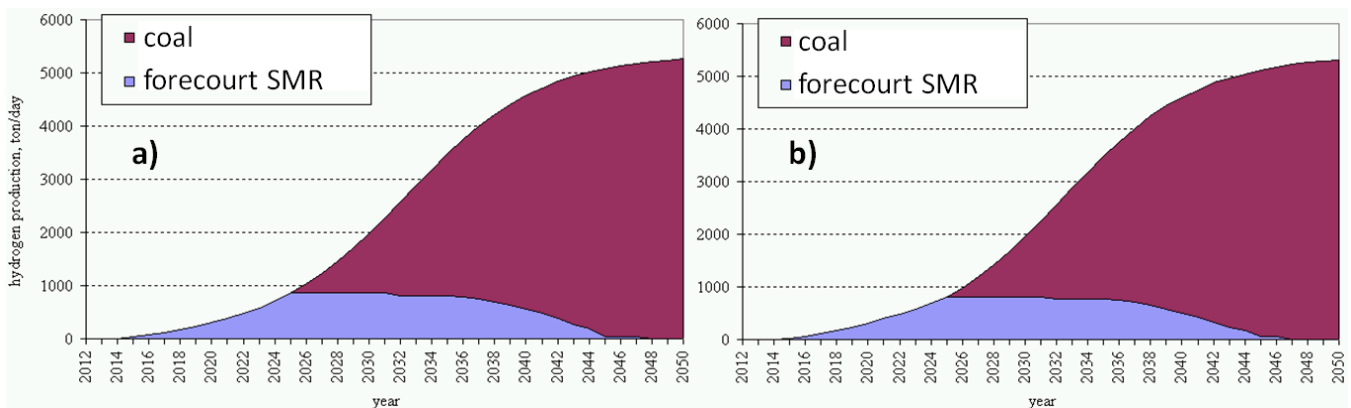


Figure 19. Cost-optimal pathways succession for a) parameterized and b) original H₂ demand curves.

Demand curve effect on hydrogen pathways

When considering more than just a generic case, different locations will require a variety of H₂ demand curves. Hence, we probe the sensitivity of the cost-optimal scenario with respect to variations in the demand curve parameters. Figure 20 shows that transition scenarios are robust with respect to demand curve variations. The parameter set that represents the original demand curve is as follows: max demand level = $1.95 \cdot 10^9$ kg/year, max demand growth rate = 0.121 1/yr, delay = 28.8 years, init rate = 0.0035 1/yr, zero years = 9.92 yrs.

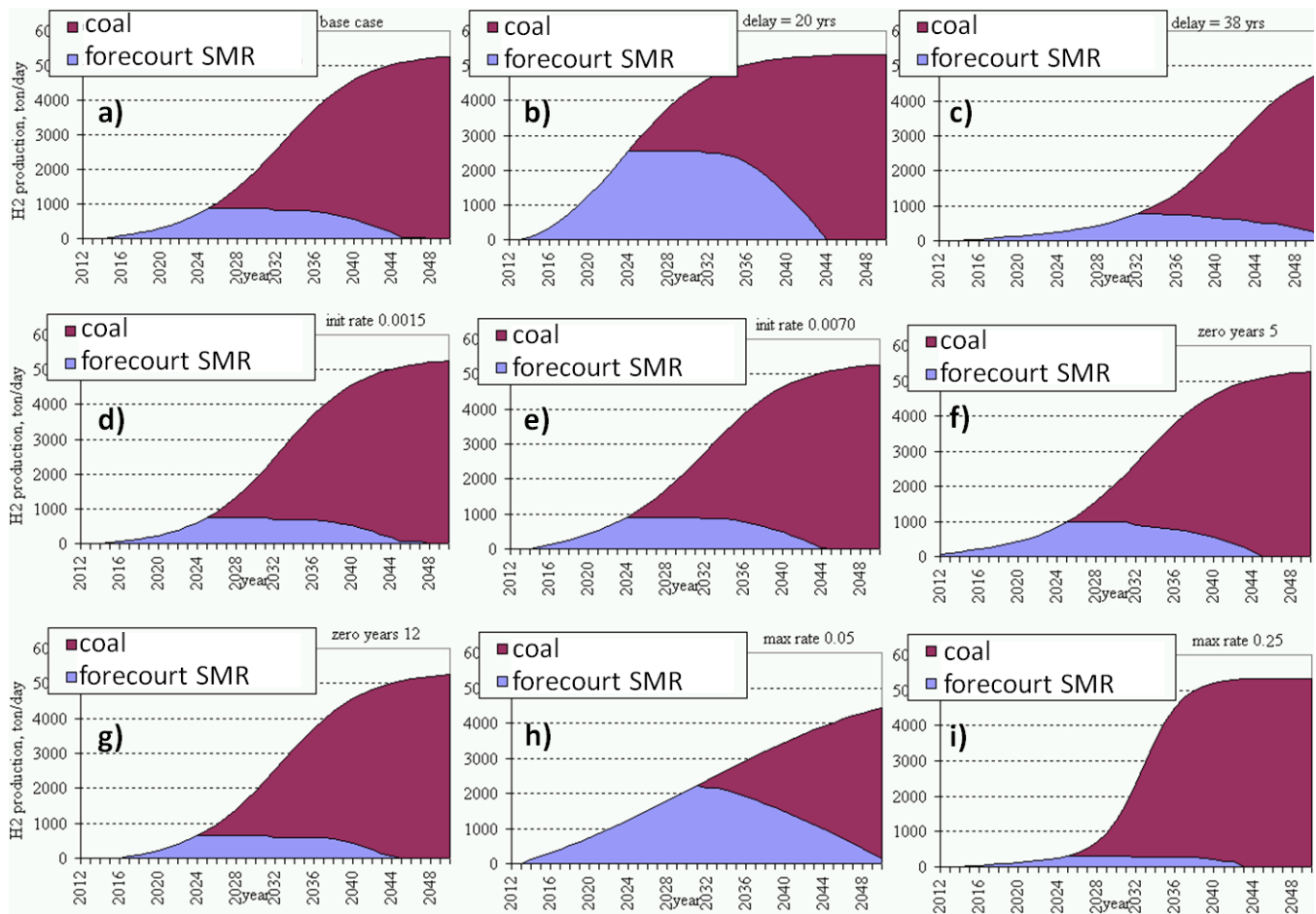


Figure 20. Cost-optimal scenarios for demand curves with a) base case parameter values; b) delay time reduced to 20 years; c) delay time increased to 38 years; d) initial rate decreased to 0.0015 yr^{-1} ; e) initial rate increased to 0.007 yr^{-1} ; f) zero years decreased to 5; g) zero years increased to 12; h) max rate decreased to 0.05 yr^{-1} ; i) max rate increased to 0.25 yr^{-1} .

Relatively large changes in the delay time (from 20 to 38 years, Figures 20b and 20c), initial demand growth rate (0.0015 to 0.007 yr^{-1} , Figures 20d and 20e), zero demand years (5 to 12 years, Figures 20f and 20g), and maximum demand growth rate (0.05 to 0.25 yr^{-1} , Figures 20h and 20i) do not incur significant changes in the succession of cost-optimal pathways. For all these cases, forecourt SMR is the cost-efficient choice during the initial demand growth years, which is replaced by coal gasification when pipeline delivery option becomes available. The year when coal gasification becomes competitive is 2025 in all cases except for delayed market development (Figure 20c) or significantly slower demand growth (Figure 20h).

The effect of the demand curve parameters on the capital costs of hydrogen pathway evolution scenarios is shown in Figure 21.

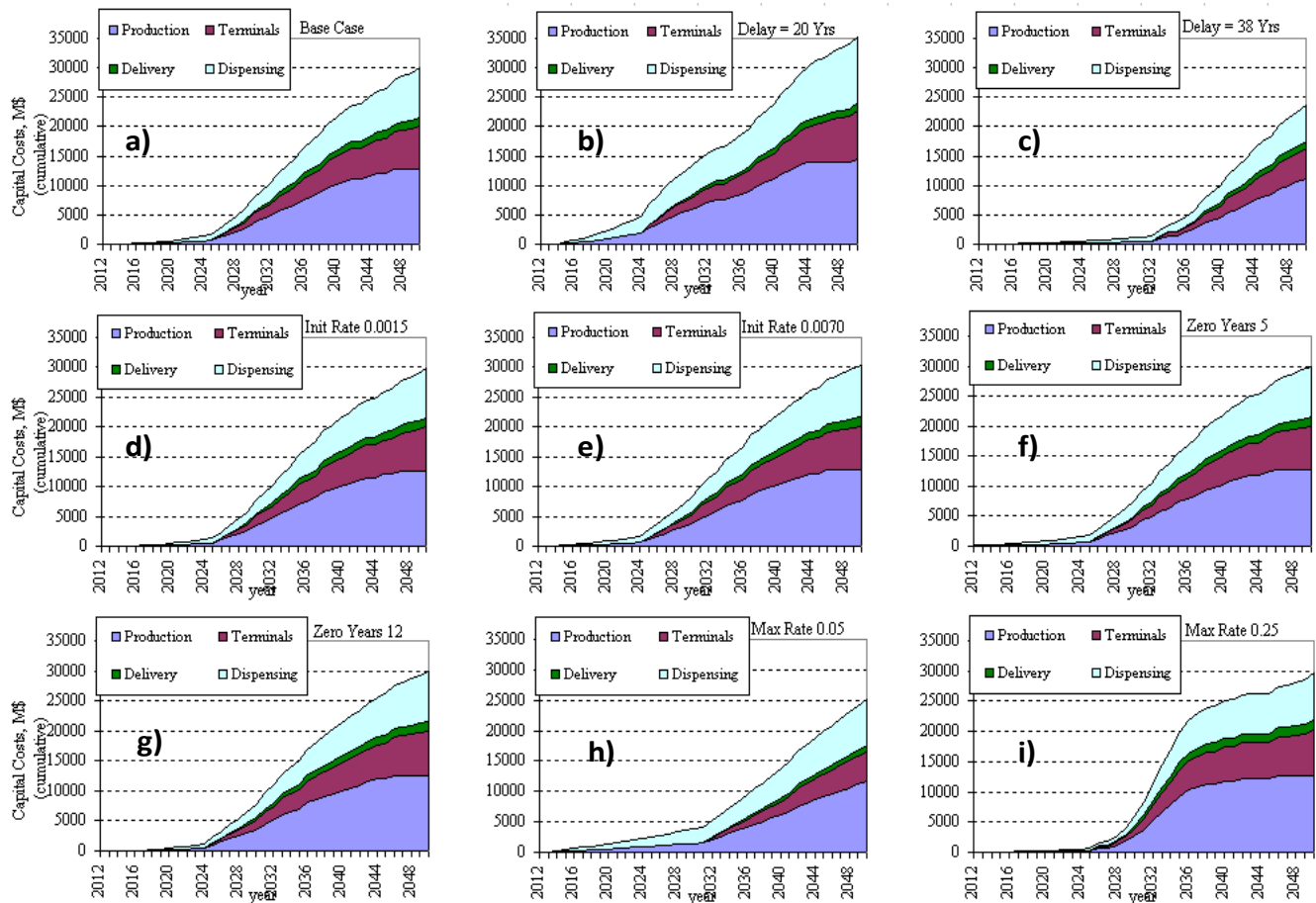


Figure 21. Cumulative capital costs of building the hydrogen infrastructure, by year, for hydrogen pathway evolution scenarios with a) base case parameter values (added for comparison); b) delay time reduced to 20 years; c) delay time increased to 38 years; d) initial rate decreased to 0.0015 yr^{-1} ; e) initial rate increased to 0.007 yr^{-1} ; f) zero years decreased to 5; g) zero years increased to 12; h) max rate decreased to 0.05 yr^{-1} ; i) max rate increased to 0.25 yr^{-1} .

Delayed H_2 demand (Figure 21c and 21h) time slows the growth of the hydrogen infrastructure, resulting in a lower accumulation of capital cost over the time period considered (2012-2050). For all other cases, the capital cost curve does not undergo significant changes. Delivery and terminal costs are associated with central production option (coal gasification). GHG emissions (Figure 22) reflect the trends discussed in connection with Figure 20.

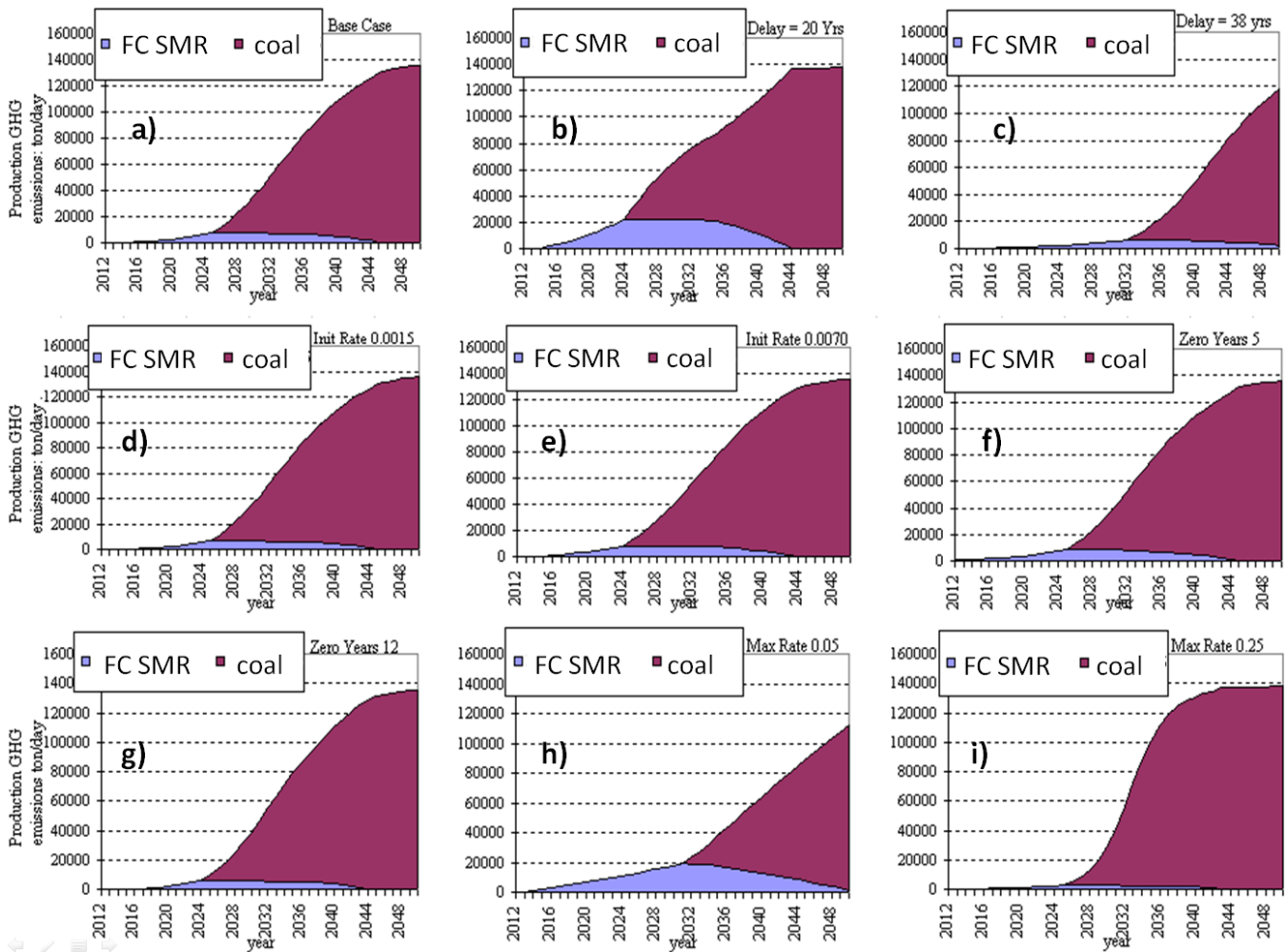


Figure 22. Production GHG emissions profiles for hydrogen pathway evolution scenarios with a) base case parameter values; b) delay time reduced to 20 years; c) delay time increased to 38 years; d) initial rate decreased to 0.0015 yr^{-1} ; e) initial rate increased to 0.007 yr^{-1} ; f) zero years decreased to 5; g) zero years increased to 12; h) max rate decreased to 0.05 yr^{-1} ; i) max rate increased to 0.25 yr^{-1} .

Further, we investigate the sensitivity of hydrogen pathway scenarios with respect to maximum demand level (which is ultimately determined by city population and hydrogen market penetration). Figure 23 shows the progression of hydrogen production pathways with respect to varying levels of maximum demand, from 0.3 to 4.0 million tonnes H_2 per year (the base case parameter value, Figure 23a, is 1.95 megaton/yr).

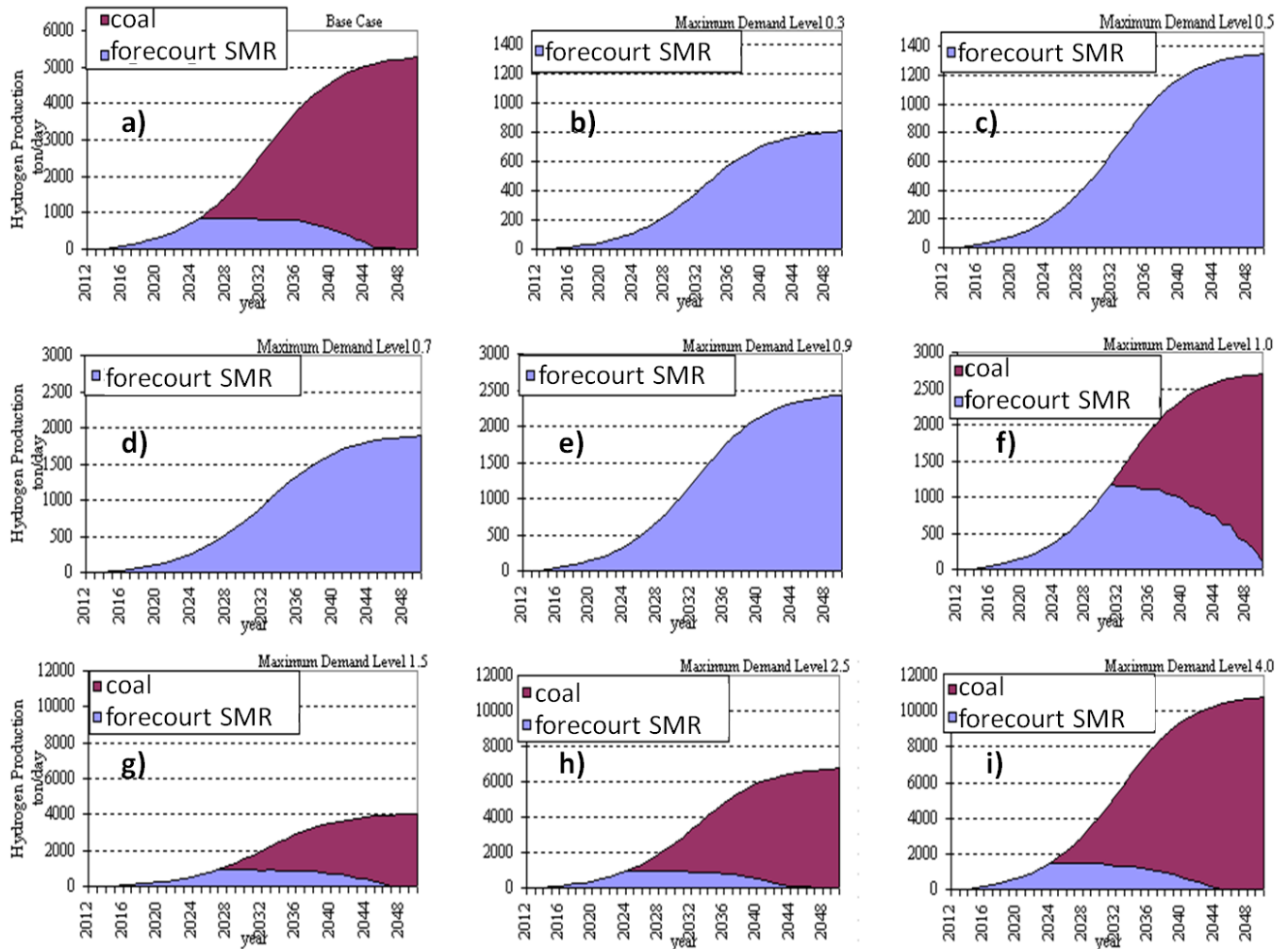


Figure 23. Hydrogen production scenarios for demand curves with maximum demand levels a) $1.95 \cdot 10^9$ kg H₂/ yr (base case) ; b) $0.3 \cdot 10^9$ kg H₂/ yr; c) $0.5 \cdot 10^9$ kg H₂/ yr; d) $0.7 \cdot 10^9$ kg H₂/ yr; e) $0.9 \cdot 10^9$ kg H₂/ yr; f) $1 \cdot 10^9$ kg H₂/ yr; g) $1.5 \cdot 10^9$ kg H₂/ yr; h) $2.5 \cdot 10^9$ kg H₂/ yr; i) $4 \cdot 10^9$ kg H₂/ yr.

As the maximum demand level changes from 0.9 to 1.0 billion kg H₂/ yr (Figures 23e and 23f), coal gasification becomes an efficient means of production around the year 2030. Further increase in the maximum demand level results in coal becoming the cost-efficient option beginning with year 2025. This transition results in a sharp increase in total capital costs (Figure 24a) and GHG emissions (Figure 24b) at maximum demand level 1.0 billion kg H₂/yr.

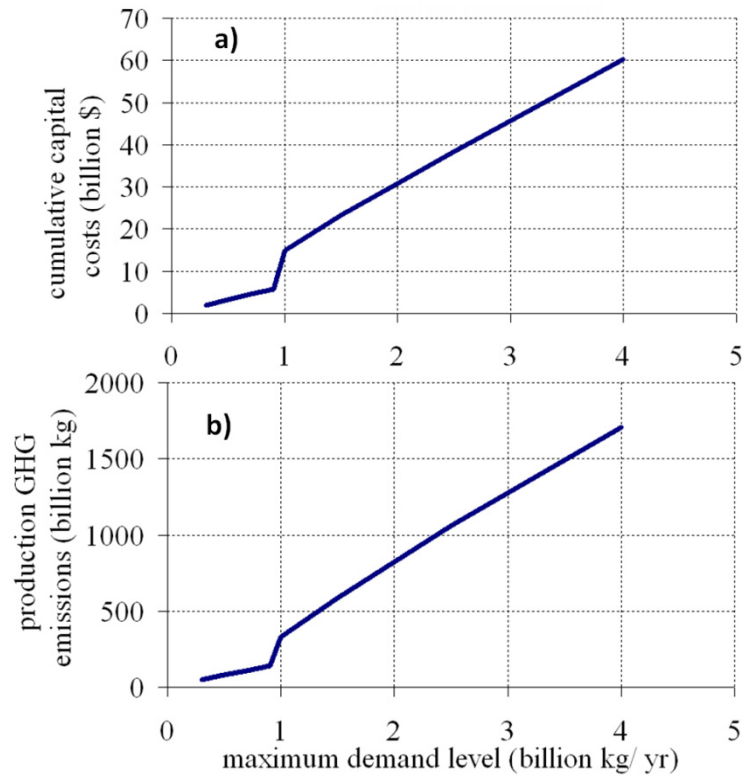


Figure 24. Total (2012 through 2050) a) capital cost of hydrogen infrastructure and b) production GHG emissions (weight CO₂ equivalent).

The transition scenario is robust with respect to demand curve variations: relatively large changes in the demand curve parameters do not affect the succession of cost-optimal hydrogen pathways. The only exception is the maximum demand level; large demand levels favor central (coal) hydrogen production over forecourt SMR in the advanced stages of FCEV market development and when the demand level is sufficiently large.

Feedstock and capital costs breakthrough points

In the course of developing hydrogen economy, well-established technologies will be combined with novel tools and this will generally exercise a downward trend on overall equipment capital costs. On the other hand, there are risks involved, inherent for new technologies or new applications of well-established processes, which might increase the capital costs of building the hydrogen infrastructure. Feedstock price volatility and geographic diversity are other sources of uncertainty. For these reasons, it is practical to know the ranges for feedstock and capital costs variation that might alter optimal hydrogen pathways succession.

Within the current study, we will limit the investigation to clean (in the sense of GHG emissions level) production technologies: biomass gasification, ethanol reforming²⁵, NG SMR with CCS, coal gasification with CCS. Potentially clean hydrogen production via electrolysis is also included (the reason behind it is that electricity can be generated almost entirely from renewable sources). We are also keeping the forecourt SMR in the mix as the competitive benchmark for comparison with cleaner technologies. First, we probe variations of feedstock prices and capital costs. Then, using a similar approach, we examine the possibilities for hydrogen production via electrolysis from (otherwise) curtailed renewable electricity.

Pathways succession sensitivity with respect to feedstock prices and capital costs

We begin with looking into NG SMR capital costs and natural gas feedstock variations that can reflect on optimal hydrogen pathways succession. At parameter values listed in Table 1 (from Generic hydrogen pathways evolution scenario), and in the absence of coal gasification (only clean technologies are considered in this section of the report), NG SMR is the cost-optimal choice. Clearly, increasing capital or feedstock costs for this production technology can result in other technologies becoming cost-favorites.

Both capital and feedstock costs in our model are time dependent. Capital costs change when advanced technology is available (in the present report, we assume new technologies become available in 2025), while feedstock costs are influenced by many factors (for example, biomass feedstock will likely grow more expensive because of land use constraints). When changing cost inputs in the model, we prefer to keep their dynamic nature. For this reason costs are multiplied by a factor. For example, if the multiplier for forecourt NG SMR capital costs is 1.1, both current (before 2025) and advanced (year 2025 and on) NG SMR capital costs are increased by 10% in the model. Similarly, biomass feedstock cost multiplier 0.8 means that biomass costs are 20% less than H2A Production default values for each year of the simulation.

Natural gas feedstock and forecourt NG SMR capital costs variation

The effects of increased capital costs of NG SMR are shown in Figure 25. Up to 70% increase in capital costs does not alter the cost-optimal pathway; in the relatively narrow interval between the capital cost multiplier values of 1.7 and 1.95, biomass gasification emerges as the less expensive hydrogen pathway for the years 2025-2030 and coal with CCS overtakes in the later years (see also Figure 26a). No changes in the cost-optimal technology before the year 2025 were observed, meaning that significantly larger changes in the cost values would be required for that.

Interestingly, increased forecourt NG SMR capital costs result in replacing it with even more capital intensive central production technologies, biomass gasification and coal gasification with carbon capture and sequestration. Naturally this becomes possible only because of relatively low biomass and coal feedstock prices (Table 1).

²⁵ Below, we do not include the analysis results for ethanol. Briefly, the feedstock price being relatively high (Table 1), no changes in capital costs for this production technology can alter the cost-optimal pathway evolution scenario.

The GHG emissions (Figure 25b) decrease significantly. A large part of the overall emissions is generated via forecourt NG SMR production (Figure 26b), while most of the hydrogen is produced by other technologies.

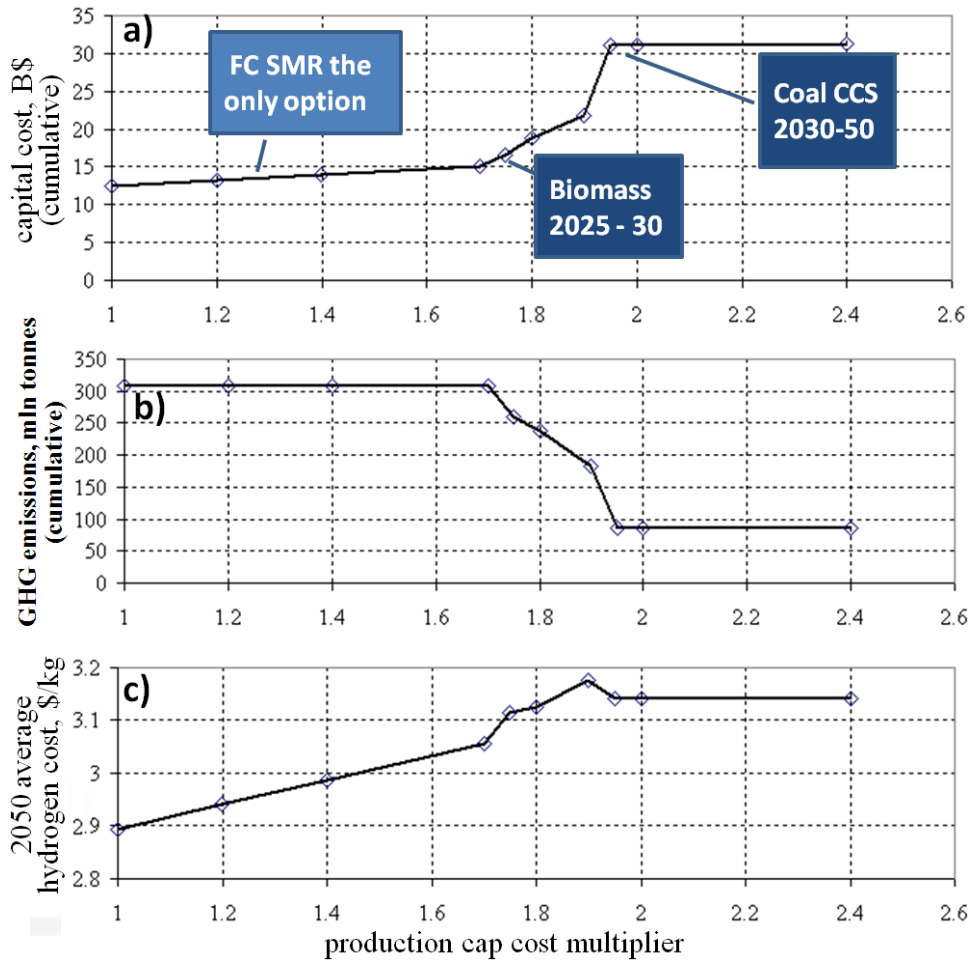


Figure 25. Forecourt NG SMR capital costs effect on hydrogen pathways evolution. a) cumulative capital costs through 2050, b) cumulative GHG emissions through 2050, c) average hydrogen cost at the pump in 2050.

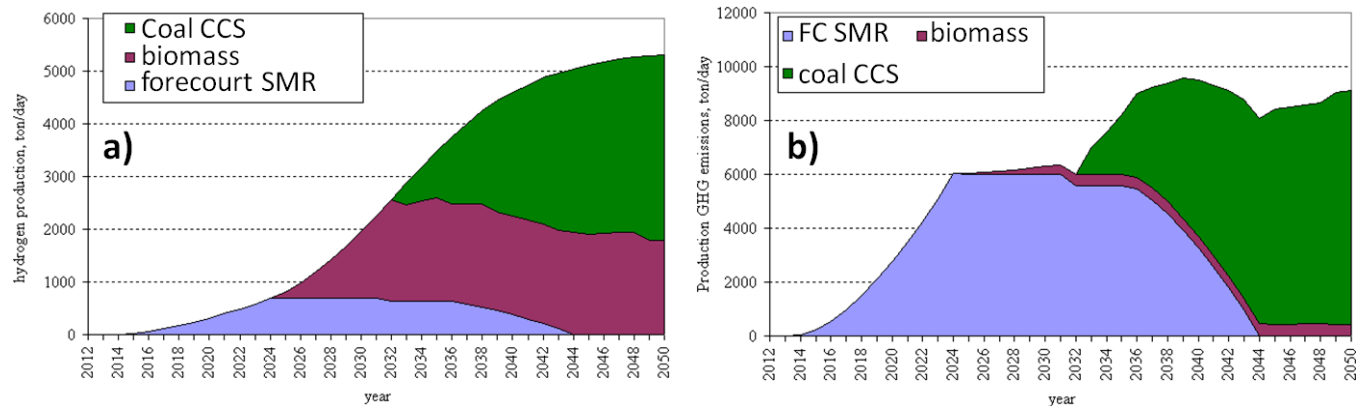


Figure 26. Cost-optimal hydrogen pathway evolution for the case when forecourt SMR capital costs are increased by a factor of 1.95. a) Hydrogen production and b) GHG emissions (metric ton CO₂ equivalent) by pathway.²⁶

²⁶ A carbon capture rate of 90% is assumed for CCS (see also Table 1)

The effect of increasing natural gas feedstock prices is similar to the effect of increasing capital costs (Figure 27): the hydrogen produced by forecourt NG SMR becomes too expensive and biomass gasification with coal CCS are preferred after the year 2025. These changes are observed at NG feedstock cost increase of 20% to 30%. The pathway evolution scenario for a 30% increase in natural gas price is identical to that shown in Figure 26 for a 95% capital costs increase. *Hydrogen pathways evolution scenario is more sensitive to feedstock price variations than to capital costs.*

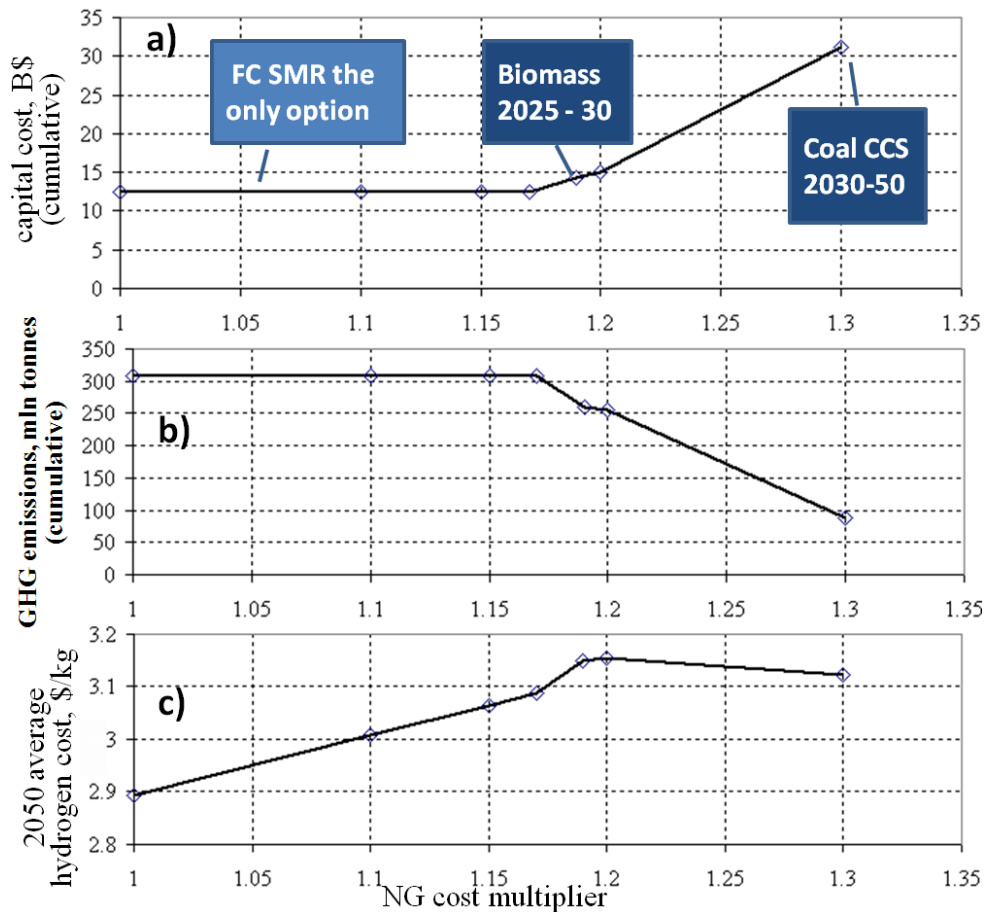


Figure 27. Natural gas cost effect on hydrogen pathways evolution. a) cumulative capital costs (billion dollars), b) cumulative GHG emissions (million metric tons), c) average hydrogen cost at the pump (dollar per kilogram).

Biomass gasification capital costs and feedstock price variation

Since biomass gasification is one of the technologies that become cost competitive upon increasing the NG SMR related costs (Figures 25-27), it is reasonable to expect that decreasing the biomass related costs will have similar results.²⁷ The biomass production option becomes competitive when feedstock cost decrease about 50% (Figure 28). Biomass gasification replaces NG SMR in the mature market (2025-2050) if feedstock is 60% less expensive than the default projections (Figure 29a). The GHG emissions are almost entirely induced by the FC NG SMR (Figure 29b), as biomass gasification related emissions are about 20 times smaller (per kg H₂ produced, see Table 1).

²⁷ Coal gasification with carbon capture and sequestration is also on the short list. We are not considering variations of coal-related costs mostly because even with CCS, this technology will emit more than two kg GHG (by weight CO₂ equivalent) per each kg H₂ produced.

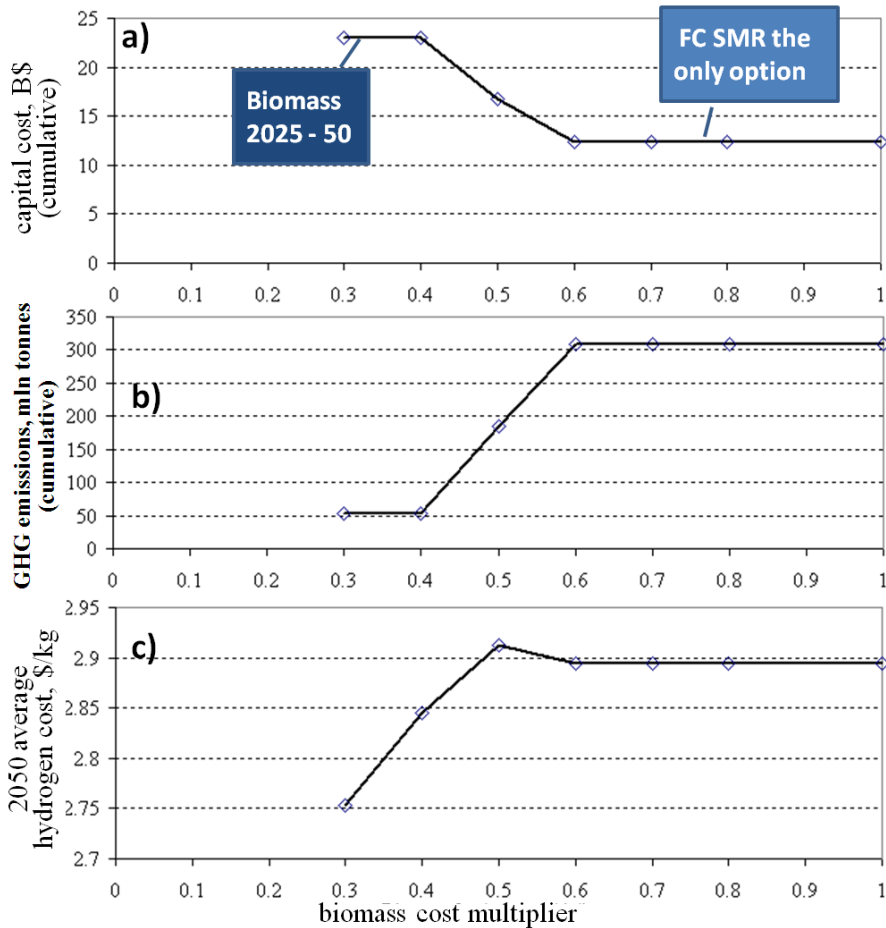


Figure 28. Biomass feedstock cost effect on hydrogen pathways evolution. a) cumulative capital costs (billion dollar), b) cumulative GHG emissions (million metric ton), c) average hydrogen cost at the pump (dollar per kilogram).

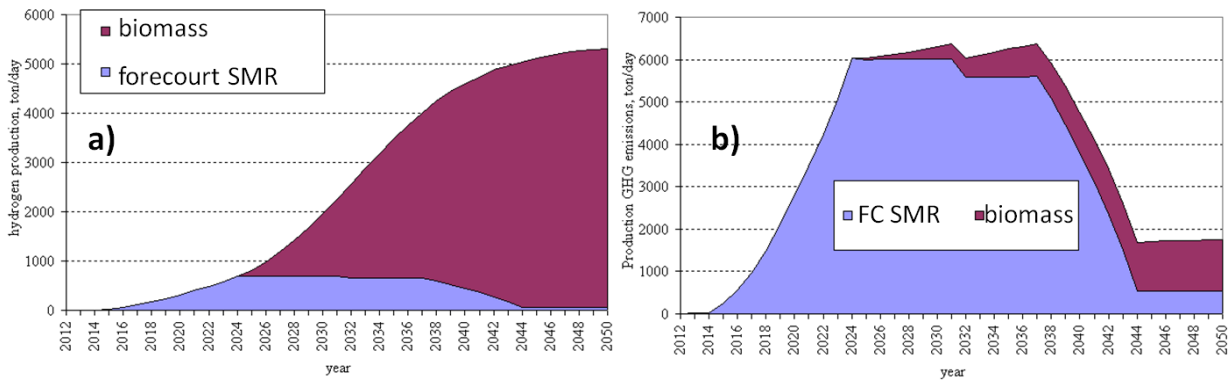


Figure 29. Cost-optimal hydrogen pathway evolution for the case when biomass feedstock costs are decreased by 60%. a) Hydrogen production and b) GHG emissions by pathway.

Decreasing biomass gasification capital costs has similar effect. With a 30% decrease, the biomass pathway becomes competitive for several years beginning with 2025 (Figure 30). However, even an 80% decrease in capital costs cannot offset biomass feedstock projected price increase – FC SMR regains its position after 2035 (Figure 31).

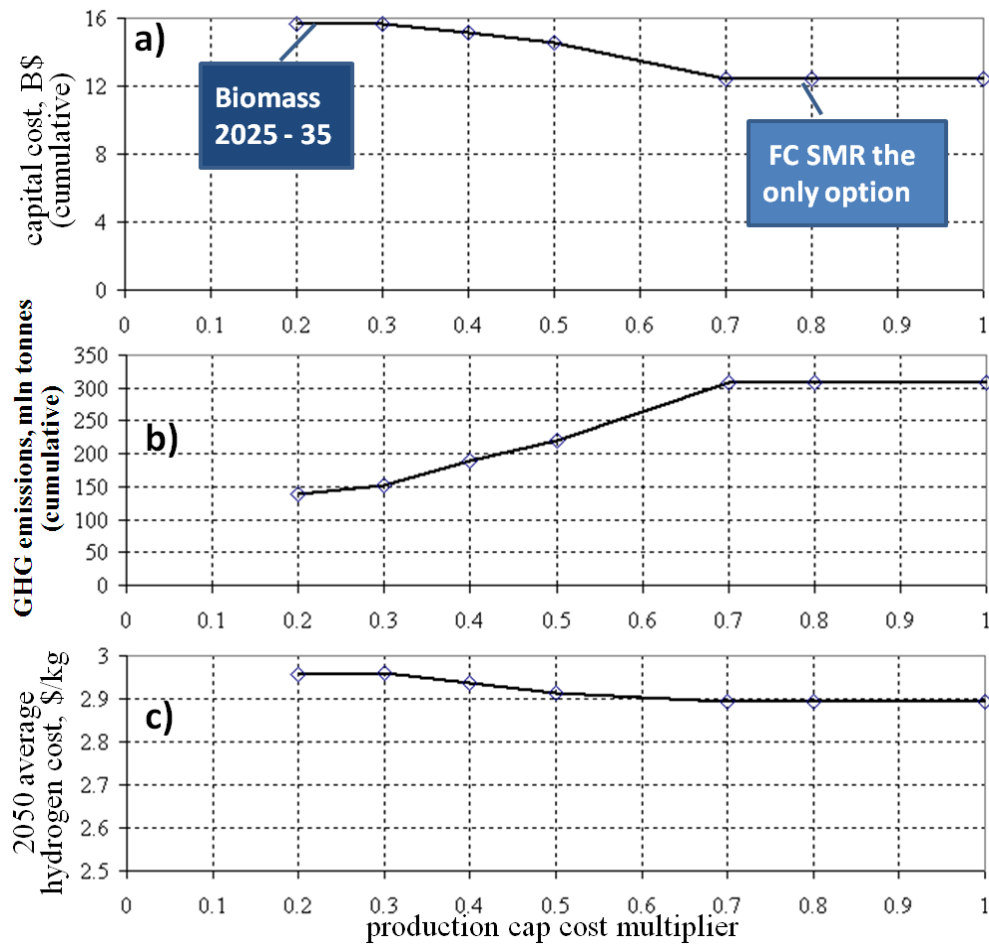


Figure 30. Biomass gasification capital costs effect on hydrogen pathways evolution. a) cumulative capital costs (billion dollars), b) cumulative GHG emissions (million metric tons), c) average hydrogen cost at the pump (dollar per kilogram).

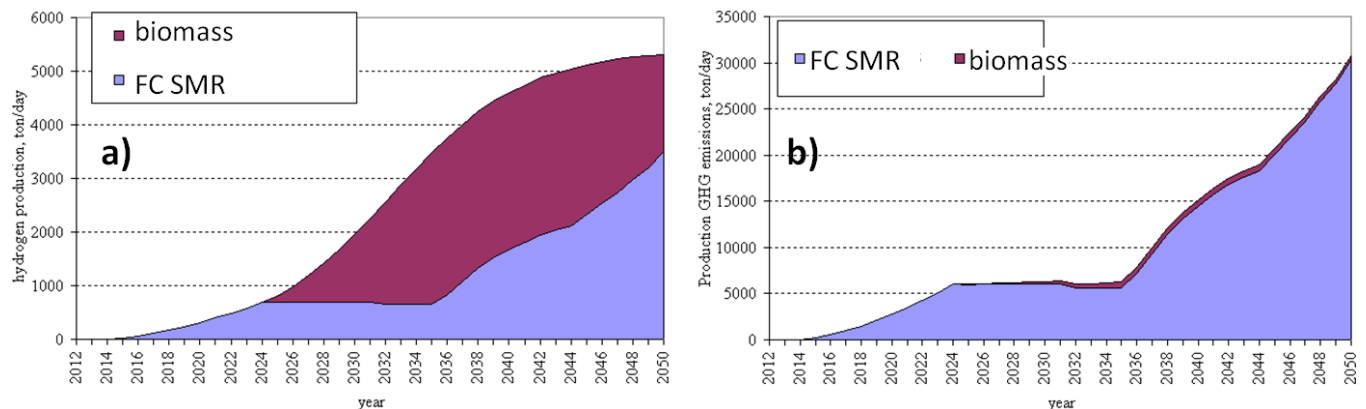


Figure 31. Cost-optimal hydrogen pathway evolution for the case when biomass gasification capital costs are decreased by 80%. a) Hydrogen production and b) GHG emissions (metric tons CO₂ equivalent/day) by pathway.

Electrolysis capital costs and electricity feedstock price variation

As mentioned above, hydrogen production via electrolysis is a potentially clean technology as long as the electricity is generated from renewable sources. Below, we find the breakthrough points for electrolysis capital costs and for electricity prices. Assuming that the transmission lines are available, forecourt electrolysis is a less expensive option than central electrolysis, because the latter also involves hydrogen delivery. Thus, we are

looking for capital cost and feedstock price levels that would make forecourt electrolysis competitive with the least expensive (and GHG emissions extensive) forecourt NG SMR option.

The model shows no cost-optimal pathway changes induced by forecourt electrolysis capital costs. The feedstock price difference between natural gas and electricity (\$1.04 vs. \$2.52 per kg H₂ produced) is too large to be offset by any capital costs reduction for electrolysis. Conversely, electricity price does affect the hydrogen pathways scenario (Figure 32). Below 50% of the default level, forecourt electrolysis is competitive with NG SMR; at the 30% of the default electricity price level, the FC Elys becomes the preferred cost-optimal choice for the years 2025-2050 (Figure 33). These changes have the potential to significantly decrease the amount of GHG emissions (Figures 32b and 33b), if low price electricity is available from renewable sources.

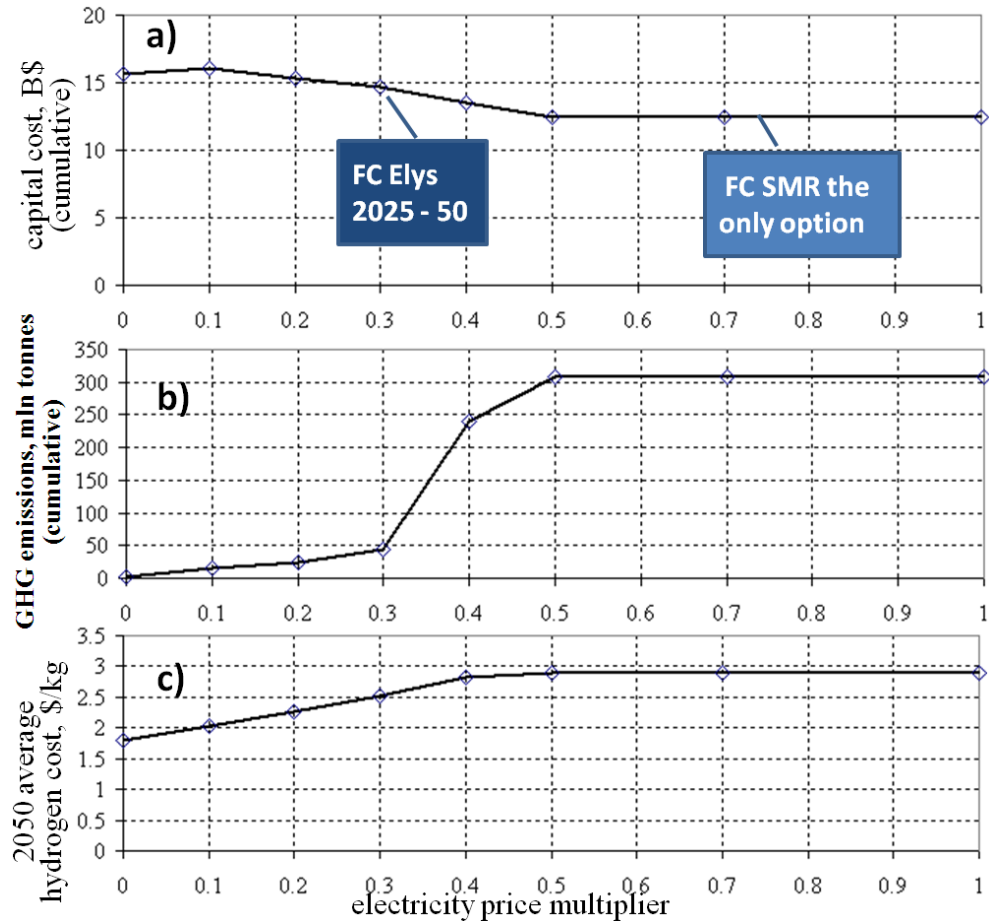


Figure 32. Electricity cost effect on hydrogen pathways evolution. a) cumulative capital costs (billion dollars), b) cumulative GHG emissions (million metric tons CO₂ equivalent), c) average hydrogen cost at the pump (dollar per kilogram).

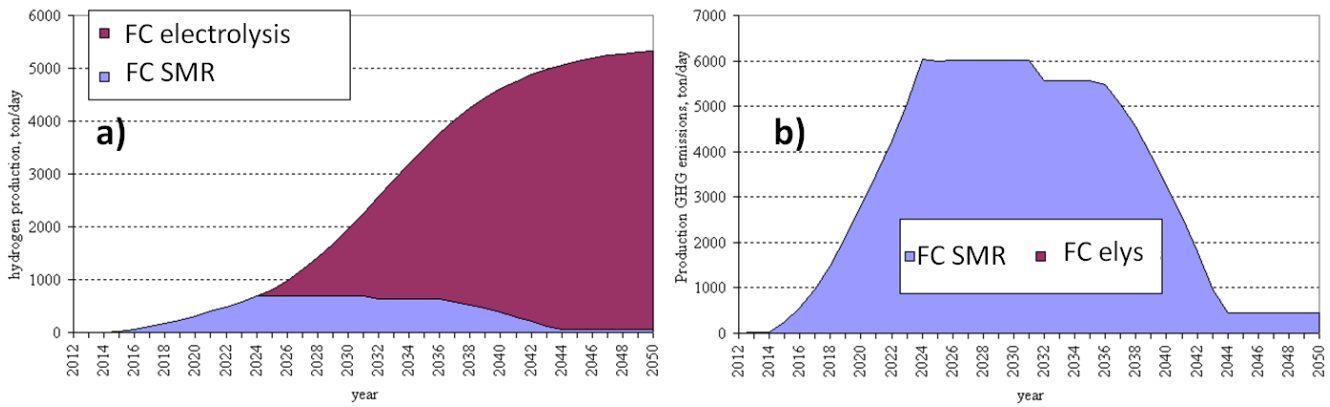


Figure 33. Cost-optimal hydrogen pathway evolution for the case when electricity price is decreased by 70%. a) Hydrogen production and b) GHG emissions (metric tons CO₂ equivalent/day) by pathway (upstream electricity GHG emissions are assumed to be zero: the electricity is generated from renewable sources).

Prospects of forecourt electrolysis using surplus renewable energy

The utilization of renewable (wind and solar) resources is subject to their intrinsic variability. If a significant fraction of power generation originates from wind and/or solar resources, for some periods of time some portion of renewable generation will be in excess of the demand and essentially free. This free electricity may be used to produce hydrogen for FCEVs. While having zero-cost feedstock electricity is a clear advantage, it still comes at a price. Because of resource intermittency, the electrolyzers will be underutilized most of the time. To account for this, we can decrease the capacity factor for the production facility. Because of the details of how HyPro organizes the interaction between various hydrogen infrastructure elements, it is more convenient to increase the capital costs instead. For example, a three-fold decrease in the capacity factor is replaced by a three-fold increase in forecourt electrolysis capital costs.

To assess the temporal characteristics of surplus electricity from renewables, the Renewable Energy Load matching model (RELM, [10]) is used. RELM accounts for all potentially available wind and solar utility scale resources [11] to match the electric power demand as close as possible. In the absence of transmission limitations, when best wind and solar resources are integrated, about 10% of the generated renewable energy is curtailed, and 35% of the time there is at least some surplus electricity. In more detail, surplus electricity characteristics are shown in Figure 34. At relatively small (compared to average wind power generation) electrolysis capacity, the electrolyzers are employed at their full capacity any time there is surplus generation (>35% of the time, Figure 34a), and that will ‘harvest’ a small part of the total surplus (Figure 34b). Increasing the capacity of electrolyzer facility will decrease the time of fully employed production capacity, while increasing total output. Below, we are investigating the competitiveness of electrolysis when ‘underemployed’ for a significant fraction of time and using free electricity.

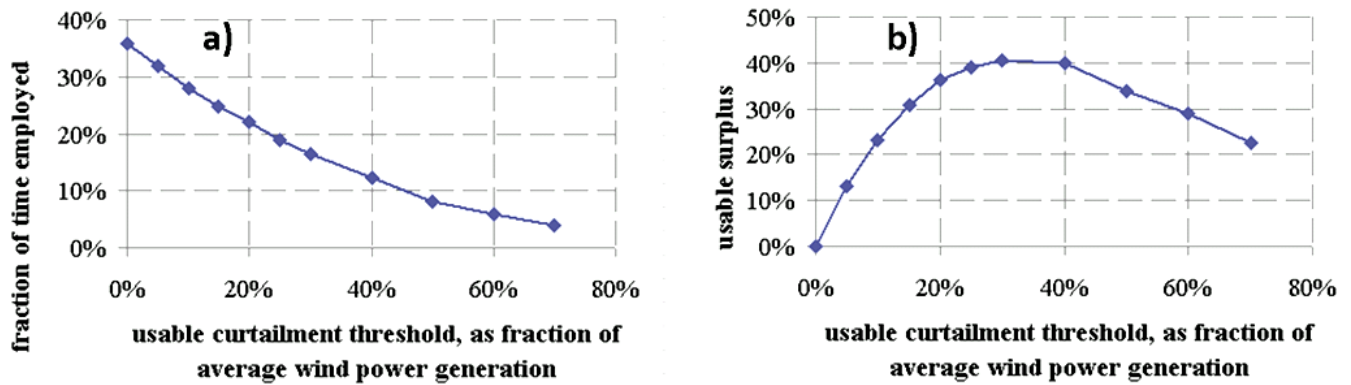


Figure 34. Surplus renewable generation: a) Fraction of time occurring and b) usable fraction of surplus energy.

It is useful to summarize the assumptions. First, the fraction of time when surplus electricity is available is calculated for ideal integration conditions for wind/solar generation sources. Including transmission limitations will likely increase the surplus generation time and reduce the underutilization of electrolyzer units. Second, capital costs of hydrogen production units are increased to account for their underutilization. Third, no hydrogen storage units (to compensate for intermittent H₂ supply) nor changing dispensing costs are considered. This assumption is likely to favor electrolysis over the forecourt NG SMR.

With these assumptions, electrolyzer units at 33% utilization (a three-fold increase in capital costs) could collect up to ~10% of the surplus electricity (Figures 34a and 34b). Forecourt electrolysis that uses surplus (*i.e.* free) electricity can compete with forecourt NG SMR in a range of underutilization values (Figure 35) spanning from 27% to 35% capacity factor.

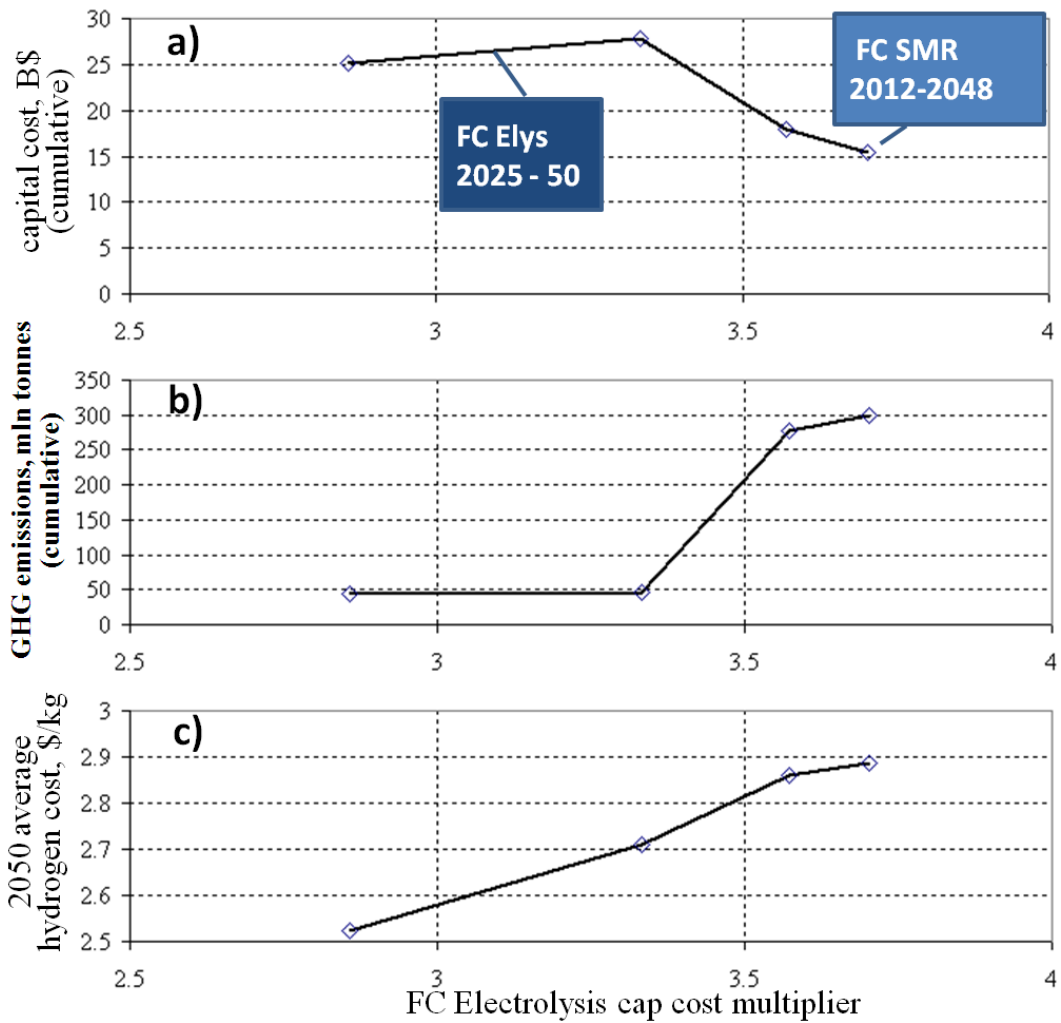


Figure 35. Forecourt electrolysis capital costs effect on hydrogen pathways evolution when using free surplus electricity. a) cumulative capital costs (billion dollars), b) cumulative GHG emissions (million metric tons CO₂ equivalent), c) average hydrogen cost at the pump (dollar per kilogram). The simulation results are shown for capital cost multiplier (horizontal axis) values 2.86, 3.33, 3.57 and 3.7 corresponding to electrolyzer units being at 35%, 30%, 28% and 27% capacity (on average over a year).

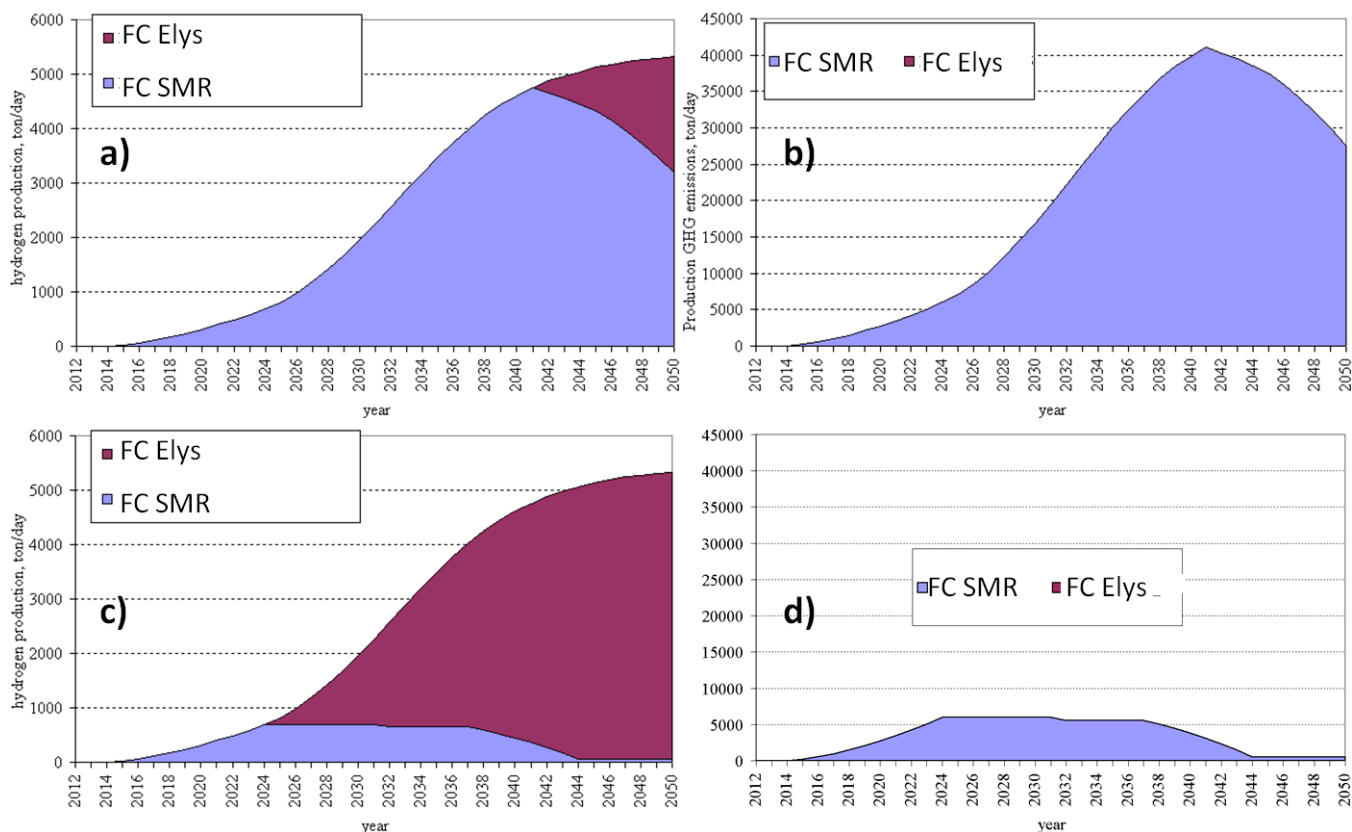


Figure 36. Cost-optimal hydrogen pathway evolution for surplus (zero cost) electricity and forecourt electrolyzer capital costs increased by a factor of (a, b) 3.57 (corresponding to electrolyzer being fully engaged 28% of the time) and (c, d) 3.33 (corresponding to 30% employed electrolyzer). a), c) Hydrogen production and b), d) GHG emissions (metric tons CO₂ equivalent/day) by pathway (upstream electricity GHG emissions are assumed to be zero: the electricity is generated from renewable sources).

When comparing clean hydrogen production technologies (biomass gasification, coal with CCS) with the most cost effective option (FC SMR), capital and feedstock cost variations capable of affecting the optimal hydrogen pathways evolution are determined. Reaching a critical parameter value leads to considerable reduction of green-house gas emissions. Several ‘tipping’ points are listed in Table 3. With respect to NG feedstock prices, a 19% increase will make biomass gasification cost-competitive. The same effect can be brought by a 30% or more decrease in biomass gasification capital costs or reducing biomass feedstock cost in half. The electrolysis from variable surplus wind electricity is competitive within a realistic range (27% to 35%) of capacity factor values.

Table 3. Critical parameter values affecting hydrogen pathways scenario

Technology	Parameter	value modification	2025 value, modified	description
FC SMR	capital costs	+75%	1.55 M\$	biomass gasification becomes competitive
	feedstock cost	+19%	7.0 \$/GJ	-“-
biomass gasification	capital costs	-30%	102 M\$	biomass gasification becomes competitive
	feedstock cost	-50%	0.76 \$/GJ	-“-
FC Elys	capital costs			no pathway changes
	feedstock cost	-60%	6.2 \$/GJ	forecourt electrolysis becomes competitive
FC Elys with wind surplus	capital costs	+270%	4.1 M\$	free surplus electricity: below 27% capacity factor, FC Elys is not competitive
	feedstock cost	-100%	0 \$/GJ	

Concluding remarks

By combining infrastructure models from the DOE suite of hydrogen analysis tools, a high level approach (HyPro – MSM) is implemented that allows one evaluate potential evolution of hydrogen infrastructure for fuel cell electric vehicles. While the infrastructure models and their inputs are validated at different levels of hydrogen analysis community, future development and deployment of new technology does present risks and unknowns.

The HyPro – MSM framework provides estimates for generic analysis of key technological inputs effects and critical ‘tipping’ points which can potentially induce large changes in the hydrogen infrastructure buildout. Green-house gas emissions and hydrogen fuel cost at the pump are the focus of this report. While presented results provide a high-level generic overview on potential effects of important technological parameters, further analysis is required to assess geographic specificity and probe the effects of other numerous parameters that might trigger significant changes in hydrogen infrastructure rollout scenarios.

References

- [1] National Academy of Sciences. 2004. The Hydrogen Economy: Opportunities, Costs, Barriers, and R&D Needs, National Academy Press, Washington, DC.
- [2] U.S. Department of Energy Hydrogen Program. <http://www.hydrogen.energy.gov/> Accessed May 31, 2011.
- [3] Ruth M., Diakov V., Genung K., Hoesley R., Smith A., Yuzugullu E. Hydrogen macro system user guide, version 1.2.1. Technical report NREL/TP-6A1-44799, July 2009. Available via <http://www.nrel.gov/docs/fy09osti/44799.pdf> [Accessed May 31, 2011].
- [4] James, B. D., P. O. Schmidt, J. Perez. 2008. Using HyPro to evaluate competing hydrogen pathways. Report on DOE contract DE-FG36-05GO15019. Available via http://www.hydrogen.energy.gov/pdfs/progress07/viii_1_james.pdf [Accessed May 20, 2011].
- [5] Steward, D., T. Ramsden, J. Zuboy. 2008. H2A Production Model, Version 2 User Guide. Technical Report NREL/TP-560-43983. Available via <http://www.nrel.gov/docs/fy08osti/43983.pdf> [Accessed May 20, 2011].
- [6] Mintz, M., J. Gillette, A. Elgowainy. 2008. H2A delivery scenario model version 1.0 user’s manual. Available via http://www.hydrogen.energy.gov/pdfs/hdsam_users_guide.pdf [Accessed May 20, 2011].
- [7] Bush, B., Melaina, M., Sozinova, O. 2010. Scenario evaluation, regionalization and analysis (SERA) model. Report on DOE contract. Available via http://www.hydrogen.energy.gov/pdfs/progress10/vii_1_bush.pdf [Accessed May 20, 2011].
- [8] U.S. Department of Energy, the office of Energy Efficiency and Renewable Energy. Multi-year research, development and demonstration plan: planned program activities for 2005-2015. Available via <http://www1.eere.energy.gov/hydrogenandfuelcells/mypp/> [Accessed May 31, 2011].
- [9] U.S. Department of Energy, U.S. Energy Information Administration. Annual energy outlook 2007. DOE/EIA-0383 (February 2007). Available via <http://www.eia.gov/oiaf/archive/aeo07/index.html> [Accessed May 31, 2011].
- [10] Short, W., Diakov, V. Large wind penetration scenarios: backup generation and energy storage requirements. Windpower 2011 Conference.
- [11] Potter, C.W., Lew D., McCaa J., Cheng S., Eichelberger S., Gruit E., Creating the dataset for the western wind and solar integration study (U.S.A.), *Wind Engineering* **32**, 325-338 (2008).

APPENDIX I. Hydrogen demand curve parameterization code

The matlab version of the computer routine used for calculating the parameterized demand curve is given below. Commentaries (green lines) show parameter values that best describe the original demand curve.

```
1 function demand = demand_curve(time_lag, max_level, init_rate, zero_yrs, max_rate)
2 %time_lag = demand_curve_params(1); % 28.8 yrs
3 %max_level = demand_curve_params(2); % 1.95e9 kg_H2/yr
4 %init_rate = demand_curve_params(3); % 0.0035 1/yr
5 %zero_yrs = demand_curve_params(4); % 9.92 yrs
6 %max_rate = demand_curve_params(5)-init_rate; % 0.121 1/yr
7
8 total_yrs = 66 ; % =length(Glo.Demand); %66
9 demand = zeros(1, total_yrs);
10 value0 = max_level / (1 + exp(2*max_rate*(time_lag-zero_yrs)));
11 for i=1:total_yrs
12     time = i-time_lag;
13     if i < zero_yrs
14         value = 0;
15         if i > 7.45
16             value = 2.05e-4 * max_level * (i-7.45);
17         end
18     else
19         ex = exp(-2*max_rate*time);
20         value = (max_level+value0)*(init_rate*(i-zero_yrs)*ex+1)/(1+ex)-value0;
21         value1 = 2.05e-4*max_level*(i-7.45);
22         if value1 > value
23             value = value1;
24         end
25     end
26     demand(i) = value;
27 end
```