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### Renewable and Sustainable Energy Reviews

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# Soft-linking of a behavioral model for transport with energy system cost optimization applied to hydrogen in EU



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#### ARTICLE INFO

#### Keywords: TIMES Energy system model Power to gas System dynamics Fuel cell vehicles Decarbonization

#### ABSTRACT

Fuel cell electric vehicles (FCEV) currently have the challenge of high CAPEX mainly associated to the fuel cell. This study investigates strategies to promote FCEV deployment and overcome this initial high cost by combining a detailed simulation model of the passenger transport sector with an energy system model. The focus is on an energy system with 95%  $CO_2$  reduction by 2050. Soft-linking by taking the powertrain shares by country from the simulation model is preferred because it considers aspects such as car performance, reliability and safety while keeping the cost optimization to evaluate the impact on the rest of the system. This caused a 14% increase in total cost of car ownership compared to the cost before soft-linking. Gas reforming combined with  $CO_2$  storage can provide a low-cost hydrogen source for FCEV in the first years of deployment. Once a lower CAPEX for FCEV is achieved, a higher hydrogen cost from electrolysis can be afforded. The policy with the largest impact on FCEV was a purchase subsidy of 5 k per vehicle in the 2030–2034 period resulting in 24.3 million FCEV (on top of 67 million without policy) sold up to 2050 with total subsidies of 84 bln $\epsilon$ .  $5 \text{ bln} \epsilon$  of R&D incentives in the 2020–2024 period increased the cumulative sales up to 2050 by 10.5 million FCEV. Combining these two policies with infrastructure and fuel subsidies for 2030–2034 can result in 76 million FCEV on the road by 2050 representing more than 25% of the total car stock. Country specific incentives, split of demand by distance or shift across modes of transport were not included in this study.

#### 1. Introduction

To have a likely probability of staying within a global warming of  $2\,^{\circ}\text{C}$  by end of this century, greenhouse gas (GHG) emissions need to be reduced by 40–70% on a global basis by 2050. Cumulative emissions need to stay between 550 and 1300 GtCO $_{2e}$  (2011–2050) whereas annual emissions today are  $\sim$ 50 GtCO $_{2e}$  [1]. This is translated into 80–95% CO $_{2}$  reduction for the European Union (EU) (compared to 1990) [2], corresponding to a less strict target of 60% for the transport sector [3] considering its more difficult nature to decarbonize [4]. In the EU, transport demand accounts for almost 33% of the final energy use (out of which road transport represents 82%) and 31% of the GHG emissions [5]. Transport is the only sector exhibiting an increase in CO $_{2}$  emissions when compared to 1990 (+23% in 2015 [6]). Strategies to reach those targets are increased efficiency, alternative fuels with a

lower  $CO_2$  footprint, modal shift (e.g. from private cars to public transport) and reduced need for travel (e.g. urban planning, home-office) [1,7,8]. There is also the need to introduce alternative powertrains in the transport sector to improve energy independence, since more than 80% of the oil is imported in the EU with an import bill of 400 bln  $\mbox{\ensuremath{\mbox{\ensuremath{\mbox$ 

The EU has adopted several initiatives to foster the deployment of alternative fuels. In the Renewable Energy Directive (RED) [10], there is a target for advanced renewable fuels (6.8% for 2030) and it has specific targets for biofuels (3.6%), but none for hydrogen. RED was revised in June 2018 [11] and includes a mandatory minimum of 14% of renewables in transport by 2030 via obligations on fuel suppliers. At the same time, conventional (i.e. first generation) biofuels EU-wide are capped at a maximum of 7%, which indirectly promotes second generation biofuels and other energy carriers like electricity, hydrogen and

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<sup>&</sup>lt;sup>1</sup> The views expressed are purely those of the authors and may not in any circumstances be regarded as stating an official position of the European Commission.

<sup>&</sup>lt;sup>2</sup> The White paper on transport has a target of 60% emission reduction target versus (vs.) 2008, while the Energy Roadmap [177] suggests 60% on average (54–67%) reduction vs. 1990. Emissions in 2008 where 33% higher than in 1990 (including maritime transport).

synthetic fuels. Electricity and hydrogen are included in the strategy of alternative fuels [12], considered as part of the deployment of alternative fuels infrastructure [13]. The new proposal of the CO₂ emission standards for the average new passenger cars and light commercial vehicles (LCV) sold in the EU post-2020 [14] defines benchmarks of 15% electric vehicle (EV) sales by 2025 and 30% by 2030 (exceeding these values will be rewarded with less strict CO₂ targets for manufacturers). There is also support in terms of financing of 70 bln€ to support low-emission mobility including 39 bln€ from the European Structural and Investment Fund, 24 bln€ from Connecting Europe Facility (in total) and 6.4 bln€ from Horizon2020 program for research activities [15]. Specifically for hydrogen, most of the EU research funding is managed via the Fuel Cell and Hydrogen Joint Undertaking (FCH JU), which is a public private partnership and has a budget of 1330 M€ (2014–2020).

Among zero emission vehicle (ZEV) market deployment, battery electric vehicles (BEV) are currently ahead of fuel cell electric vehicles (FCEV). On a global level, there are over 5.1 million EV (BEV and plugin hybrid electric vehicles (PHEV)) [16], while there are only close to 11200 FCEV on the road [17]. How these powertrains compare in the future will depend on the learning achieved by deployment. With learning rates of 6-9% [18] or even 16% [19], lithium-ion EV batteries could reach a cost between 50 and 75 €/kWh by 2040 [19,20], while fuel cell cost could be reduced from 233 €/kW³ to an ultimate cost of 25 €/kW [21]. While the most affordable BEV in the C segment are being sold for around 30-35 k€ (plus VAT) [22], FCEV sales are currently dominated by a single model (the Toyota Mirai on the D segment) marketed in Germany at 78.6 k€ [23]. Specific energy consumption is better for BEV (0.33 MJ/km vs. 0.63 MJ/km for FCEV [24,25] with a wider difference for long distance [26] or when the entire pathway is considered [27]). Both powertrains have limitations, driving range and charging time are the main issues for BEV, while fuel cell cost and lower efficiency are issues for FCEV [22]. A possible complement between both is to use BEV for short driving range and smaller vehicles size, while FCEV are used for longer distances and larger cars [21].

Another key barrier for both powertrains is infrastructure. By end of September 2017, there were over 120000 publicly accessible recharging points for EV in the EU, of which almost 15000 were fast charging [28]. In contrast, only 82 hydrogen refueling stations are in operation in the EU [28,29]. The EU directive (2014/94/EU) specifically addresses the need for infrastructure deployment of alternative fuels [29]. An assessment of the national policy frameworks submitted as part of this directive, indicates that the investment needed is almost 900 M€ for electricity by 2020 and 700 M€ for hydrogen by 2025. This would be on top of 3.9 bln€ by 2020 for 440000 public accessible recharging points and an ambitious target of 4 million EV on the road [29].

There are multiple ways to model transport at different spatial and temporal scales from agent-based, system dynamics, engineering and integrated assessment models [30]. System dynamics (simulation) usually focuses on the transport system and stakeholders interactions, while cost optimization usually disregards factors like budget (or income), time availability, preferences and risk aversion, that also influence decisions [31,32]. This study soft-links these two types of models, combining their strengths and making trade-offs across the entire energy system [33–35]. The specific models used are JRC-EU-TIMES<sup>4</sup> which covers CO<sub>2</sub> emissions from the energy system and allows assessing the effect not only of technology assumptions (e.g. electrolyzer efficiency and cost), but also the effect that systemic parameters (e.g. CO<sub>2</sub> underground storage) have on cost and commodity prices. JRC-EU-TIMES has been used in the past to assess the parameters that promote and hinder hydrogen use in alternative future scenarios [36]. The other

model is Powertrain Technology Transition Market Agent Model (PTTMAM) which has 4 market agent groups (manufacturers, users, infrastructure providers and authorities) and has been used in the past to assess scenarios for the road transport sector [37] and provide policy insights [38,39]. In both cases, the geographical scope is the same (EU28) and they are used for the time horizon of 2050, when the shares for FCEV are expected to be the highest.

The reason to focus on FCEV is twofold. First, from a purely economic perspective, the case for FCEV is more difficult to justify (compared to BEV), so applying a system dynamics model that covers noncost related attributes will shed light into the potential role FCEV can play when considering a more holistic evaluation. Second, transport has one of the highest willingness to pay for the hydrogen given its higher difficulty to decarbonize [40,41]. This will help to justify the potential investment in hydrogen production and facilitate the integration of variable renewable energy (VRE) [42] (when produced through electrolysis). The hydrogen potential for transport extends beyond cars. When converted to other energy carriers such as ammonia or liquid fuels, it can satisfy demand in aviation or the maritime sector [17]. Even within the road transport sector, hydrogen can be attractive for heavy-duty long-haul trucks and buses that have higher power requirements (leading to larger batteries if BEV are used). However, given that the fuel choice for these sectors is fundamentally different from cars, this study focuses specifically on passenger transport.

Based on this, the main objective of this study is twofold: (1) assess how soft-linking affects the stand-alone output of each model; (2) quantify the effect that different policies and subsidy schemes can have in FCEV penetration and the cost effectiveness of these policies. The main novelties are: (1) the soft-linking of the two mentioned models with complementary features; (2) the coverage of the entire EU (rather than one country); (3) the use of ambitious CO<sub>2</sub> targets and (4) analyzing the effect different policies can have on FCEV penetration. Some of the questions to be answered are: how does the soft-linking process affect total system cost and commodity prices, what are the system drivers that favor FCEV, what actions are needed (from the manufacturers, authorities and infrastructure) to promote FCEV deployment, what is the incentives scheme (amount and timing) required to increase the FCEV share, how does R&D subsidy compare with vehicle and financing of refueling stations.

The rest of the paper is organized as follows. The next section presents a literature review and identifies gaps in the literature. Section 3 describes the methodology and modeling approach. Section 4 covers the data and assumptions, while Section 5 goes through the scenarios and policies evaluated. Section 6 presents and discusses the results and lastly Section 7 summarizes the conclusions.

#### 2. Literature review and gaps

This section is split in various clusters where each one looks at a different element of the present study: 1. Use of stand-alone system dynamics models for alternative fuel vehicles and specifically for FCEV; 2. Use of stand-alone optimization models for hydrogen use in lowcarbon systems; 3. Incorporation of the behavioral component in integrated assessment models; 4. Incorporation of the behavioral component in energy system models. This literature review does not cover studies for the hydrogen supply chain (commonly referred as HSC) or specific geographical match between sources (e.g. high renewable potential locations) and sinks. As starting point for that discussion, refer to Refs. [43,44] for a review of the different models, [45] for UK or [46-48] for Germany. Other approaches to model diffusion of alternative fuel vehicles including agent-based modeling [49], computable general equilibrium [50] and econometrics (usually suitable for shortterm forecasts) have been left out of the review since they use a different modeling approach. For a review of applications of these other approaches to BEV, refer to Ref. [51].

 $<sup>^3</sup>$  Throughout this report a currency conversion of 1 € = 1.2 \$ has been used.  $^4$  TIMES = The Integrated MARKAL-EFOM System; MARKAL = Market Allocation; EFOM = Energy Flow Optimization Model.

 Table 1

 System dynamics models applied for FCEV penetration.

Model	Region	Soft-linking	Findings	Gaps	Reference
HyDIVE	California	z	Highly non-linear thresholds for tax credits, subsidies and intangible costs were identified beyond which FCEV and refueling stations is self-sustained. Clustering of refueling stations around metropolitan areas.	Alternate transition strategies. Better quantification of the level and duration of subsidies. Evaluation of different spatial distributions of initial hydrogen refueling stations. Improved understanding of the effect of various rechnoloxy performance and rost parests	[56]
H <sub>2</sub> VISION	Generic/Washington D.C	z	A coordinated policy approach to promote FCEV sales in parallel to infrastructure development is the most effective measure for FCEV adoption.	Consider other agents besides infrastructure. Introduce heterogeneity for consumers. Include additional attributes for consumer choice.	[57]
ASTRA	EU25 + NO + CH	Y – With a hydrogen transition model	It is used with market penetration from HyWays project, focused on Germany and assesses the impact of limited subsidies, infrastructure development and hydrogen fuel taxing, where failure of any of these three measures results in failure of significant FCEV penetration (especially the first two).	Include a sensitivity analysis for FCEV performance. Exogenous FCEV share. Exogenous learning curve for fuel cell.	[58]
FCEV Transition Model	Germany	z	ded to ensure that FCEV reach one third of the equivalent to the CAPEX difference with ICEV infrastructure deployment (500 stations for emption (until the first million vehicles is cumulative budget deficit of 4.8 blnc.	Focused only on hydrogen and no competition with other powertrains. Exogenous fuel price assumption. Exogenous learning curve for fuel cell.	[59]
1	us	Z	Multiple equilibrium levels are possible for the alternatives, meaning that certain value thresholds must be met for the alternatives to penetrate the market. Small differences in infrastructure development can make a big difference for penetration of alternative fuels.	Use of alternative data and assumptions. Introduce more technologies. Consider multiple regions. Creation of an interface. Alternative plausible scenarios.	[09]
1	Korea	z	yzed that ding Financing	Introduce heterogeneity for consumers. Additional attributes for consumer choice. Include a sensitivity analysis for FCEV performance. Exogenous learning curve for fuel cell.	[61]

#### 2.1. System dynamics models for FCEV

System dynamics models have been applied to various areas of transport including uptake of alternative fuel vehicles, supply chain management, highway maintenance and construction, air travel and urban planning [52]. For alternative fuels, they have been used to evaluate the penetration of EV in the Netherlands and UK [38], Compressed Natural Gas (CNG) in Switzerland [53] and biofuels in US [54] and EU [55]. The applications for FCEV are limited and these are reflected in Table 1.

Some of the gaps these previous studies have in common that the current one will cover are: (1) consideration of other market players (like providers of refueling stations and manufacturers) that also play a role in influencing FCEV penetration; (2) the consideration of the rest of the energy system and how updated demand affects prices (through soft-linking with the energy system); (3) cost effect of FCEV and hydrogen refueling stations on total system cost; (4) endogenous cost development as a function of both deployment and choices made by car manufacturers.

#### 2.2. Energy system models for hydrogen and FCEV

Hydrogen is a common topic studied with energy system models [46,47,62–87]. With the potential use in FCEV, hydrogen for transport was one of the first hydrogen applications and in some cases the only one evaluated. With stricter CO2 targets and a potential "hydrogen economy" [46,88,89], uses in other sectors started to be included. While most of the studies focus on the (now) conventional application of FCEV penetration, some studies go a step further and have an additional element in one of two directions: 1. Higher spatial resolution to match supply (e.g. high renewable energy sources) and demand centers (e.g. cities) and have a better estimate of the infrastructure cost to connect these two [46,73,82,90]; 2. Including intangible costs (like range anxiety, refueling stations, model availability) that influence the choices made by consumers when selecting a powertrain in an attempt to improve the initial optimization based purely on cost [91]. There are examples for Germany [47,79,80] with both high spatial and temporal resolution that determine the best locations for hydrogen production (using power surplus from VRE) and the amount available (based on hourly profiles). These still lack the energy system perspective, where demand from all sectors is considered in competition for the hydrogen produced, effect on prices and endogenous calculation of the hydrogen demand. Taking as starting point energy models that have looked into hydrogen and then added more details, the most advanced examples can be seen in California with a combination of ambitious CO2 and ZEV targets and in the UK. Both of these are briefly explained below.

CA-TIMES [81,92–94] is managed by the Policy Institute for Energy, Environment and Economy at UC Davis [81]. looks at hydrogen delivery pathways including distance and flow for transmission and population density and market penetration for distribution. It uses such detailed analysis to update TIMES. Another boundary that has been partially crossed is the behavioral one, where [91] has taken output from MA3T and fed it back to TIMES through introducing: more segments in the market, an inconvenience cost for refueling infrastructure (additional distance to be traveled to fuel the vehicle), range limitation cost, risk attitude and consumer heterogeneity. Follow up work included even a finer segregation by introducing clones within a market segment (20 clones for each of the 36 segments) that capture randomly distributed unobservable differences in preferences [95]. A proof of the compromise and complexity associated to combining different complementary approaches is that this version of TIMES is extended to cover the spatial component by splitting California State in 8 different regions to determine the specific production technologies, delivery pathways and hydrogen demand in time [96,97]. However, such version is treated as a separate model (H2TIMES [82]) and does not capture the interaction with the other sectors in the energy system.

In the case of UK, projects requiring an energy modeling component use UCL MARKAL. It has over 35 years of history as preferred tool to provide advice on national energy policy [98]. The hydrogen system was developed in two stages, as part of each phase of the UKSHEC (United Kingdom Sustainable Hydrogen Energy Consortium<sup>5</sup>). As part of the effort to improve the transport representation, additional technologies were introduced leading to a finer market segmentation, incorporating the supply chain and infrastructure from previous studies and using a lumpy investment option<sup>6</sup> [99]. The revised model resulted in 99% penetration of hydrogen cars by 2050 with an 80% CO<sub>2</sub> reduction, which was compared to other studies in UK [90]. The softlinking with a simulation model (UKTCM<sup>7</sup>) has also been done where the feedback to MARKAL was the demand (fixed activity) and efficiency for each type of car, excluding the elasticity effect in MARKAL which was already included in UKTCM [100].

The range of studies that have used energy system models to assess hydrogen potential as energy carrier are shown in Table 2 highlighting the ones that have looked beyond transport and the ones that have included either a higher spatial resolution for infrastructure or the behavioral component.

The main gap covered in this study compared to previous ones is the consideration of some of the intangible costs that also affect the consumer decision and additional market agents besides the consumers themselves that can either promote or limit FCEV penetration.

#### 2.3. Incorporation of behavioral aspects of transport in IAM

FCEV have also been evaluated with Integrated Assessment Models (IAM). The added value (for this study) of looking at IAM is that since they cover a wider set of modules, they also need to simplify the representation of the transport sector to avoid a highly complex model. IAM differ from energy system models since they also include land use, agricultural, forestry, macro-economy and climate modules and they have a global scope [105]. To improve the representation of the transport sector, mainly two features have been introduced (the same as with energy models): one is a higher segregation of the consumers, fine enough to represent different socio-economic groups that will have a different perception and weights for the attributes when choosing a specific vehicle. The other one is monetization of intangible costs that are usually not considered in cost minimization tools such as range anxiety (in the case of BEV), refueling station availability (for early stages of infrastructure development), risk premium (to represent perception of new technologies risk), model availability (in early stages) and BEV chargers [32]. Only recently, these behavioral features have been introduced and more time is needed for it to become widely adopted. Heretofore, IAMs have been used in the conventional way to assess FCEV penetration (see Table SI 1 in Appendix 1) usually with logit functions for the market shares and with elastic demand that is sensitive to fuel prices and only some of them include modal shift. With respect to FCEV some limitations that arise are: some IAMs do not have hydrogen as option for passenger vehicles (e.g. WITCH [4]) or do not have endogenous learning linking cost reduction to FCEV deployment (e.g. GCAM [4]), establish a maximum share that FCEV can acquire or have limited representation of the infrastructure (critical for both BEV and FCEV). In spite of this, most of them show that hydrogen does not play a role (< 5%) by 2050 and only under strict (450 ppm CO<sub>2</sub>) scenarios, it becomes a significant energy carrier for transport by 2100

 $<sup>^{5}\,\</sup>mathrm{From}$  2003 to 2007 and funded by the Engineering and Physical Sciences Research Council.

<sup>&</sup>lt;sup>6</sup> The model chooses to invest in infrastructure with a minimum size (to ensure a minimum threshold is passed to deploy infrastructure).

<sup>&</sup>lt;sup>7</sup> UK Transport Carbon Model covering vehicle ownership, travel patterns, fuel efficiency (driving style), vehicle ownership, stock turnover and valuation of external costs, among others.

**Table 2**Energy models used for hydrogen potential assessment for different geographical regions.

Region	Model	H <sub>2</sub> use <sup>a</sup>	Infrastructure <sup>b</sup>	Behavioral component	Application	Reference
Belgium	MARKAL	R,P,T,Ref	No	No	Hydrogen potential (with focus on transport)	[72]
California	CA-TIMES	T	Yes	Yes	FCEV penetration, infrastructure development	[81,82]
Canada	TIMES-Canada	T	No	No	BEV penetration	[83]
China	MARKAL	T	No	No	FCEV penetration by 2045	[85]
China	China-TIMES	T	No	No	Transport sector with 10, 20 and 50\$/ton (CO2 price)	[86]
Europe	REACCESS	R,C,I,P,T	No	No	Hydrogen potential for transport	[101]
Europe	JRC-EU-TIMES	R,C,I,P,T	No	No	Current policies and 80% CO2 reduction by 2050	[87]
Germany	MOREHyS (Balmorel)	P,T	Soft linking	No	Hydrogen role and link with GIS	[46]
Global	GMM	T	No	No	FCEV role and promotion linked to a climate model	[62]
Global	TIAM-ECN	T	No	No	H <sub>2</sub> potential for Europe	[64]
Global	GENeSYS - MOD	T	No	No	1.5 °C scenario for 2050	[102]
Italy	MARKAL-Italy	R,P,T,Ref	No	No	Hydrogen role in future system	[65]
Japan	MARKAL	T	No	No	FCEV penetration	[66]
Japan	METANet	T	No	No	FCEV penetration	[67]
US	MARKAL EPA US9R	T	No	No	FCEV penetration	[68,69]
UK	UK MARKAL	R,P,T	Yes	Yes	FCEV penetration, infrastructure development, residential FC	[70,71,103
Norway	TIMES-Norway	T	Soft-linking	No	Coupling with infrastructure	[73]
Scandinavia	Balmorel	P,T	No	No	H <sub>2</sub> role in the transition to a low carbon transport	[74,104]
Spain (Madrid)	MARKAL	T	No	No	FCEV share for 3 scenarios for 2050	[75]
Switzerland	MARKAL	T	No	No	Lower primary energy consumption	[76]
Switzerland	STEM (TIMES)	T	No	No	FCEV penetration	[77]
South Africa	TIMES-GEECO	T	No <sup>c</sup>	No	Transport emissions and energy demand	[78]

<sup>&</sup>lt;sup>a</sup> This refers to the sectors where the model has the choice of using hydrogen; R = Residential; C = Commercial; I = Industry; P = Power; T = Transport; Ref = Refinery.

[7,106,107]. In some cases [106,108], carbon capture and storage (CCS) also becomes critical since it is the main route used to produce (and decarbonize) the hydrogen.

## 2.4. Incorporation of behavioral aspects of transport in energy system models

There are three main features that have been introduced: modal shift, consumer heterogeneity and use of intangible costs. A set of studies [109,110] looked into incorporating modal shift by introducing new parameters such as travel time budget, monetary budget, speed of the different transport modes, infrastructure requirements (e.g. bike lanes) and additional constraints such as maximal modal shares and maximal rate of shift. This is also linked to the demand split by distance traveled to be able to account for the different time variation in case of choosing an alternative transport mode. The aim of introducing travel time in a cost optimization framework is twofold: (1) It enables the use of more expensive modes of transport that are able to reduce traveling time; (2) It relates the investment in infrastructure to a reduction of travel time of public transport modes.

Additional efforts have been made to split demand further and account for its heterogeneity with different characteristics (e.g. income) and attributes evaluated by the different types of consumers [91,111]. Particularly in Ref. [111] the split is made based on region, type of residential location (urban, suburban and rural) and income level, which has resemblance but yet different from the split chosen for IAM (residential location, distance traveled and attitude toward technology adoption). To exploit this demand segregation and the different weight each one gives to each attribute, additional intangible costs are introduced including refueling infrastructure, range limitation (for BEV), risk attitude and model diversity [91]. In every case, this requires the collection of additional data (e.g. number of trips per person, average trip distance, travel time for public transport, average speeds by distance, load factors for cars, infrastructure utilization) to be gathered. In the case of California and Denmark [91,111], there was a highly disaggregated simulation model for the transport sector (regional models which had respectively over 1450 consumer segments and over 1200 zones) that contained all the information necessary to introduce both

the modal shift and the intangible costs. For the case of Ireland [110], mostly national sources of statistics were used. Since the present work has a wider geographical scope (EU28), there is no single source that has consistent input in terms of market segmentation, demand split by distance, mode of transport and growth in time. Therefore, a simulation model (PTTMAM) is used where the trade-off has been wider geographical coverage at the expense of focus only on the passenger car market without modal shifts.

There are two examples of soft-linking an energy model based on cost optimization with a simulation model [25,112]. One [25] was for Ireland, using TIMES and a model for the car stock evolution based on activity, stock composition, energy intensity and emission factors where the choice of future sales was based on a combination of income and fuel elasticities. The possibility of an 80% CO $_2$  reduction by 2050 (vs. 1990) was explored. Three measures were analyzed: improved energy efficiency (75 gCO $_2$ /km by 2050), level of biofuel blending and degree of reduction of intangible costs for alternative vehicles (i.e. BEV). The other one [112] focused on France and Germany for 2030, while also using a Pan-European TIMES to assess the powertrain mix for 2050 with 80–90% CO $_2$  reduction scenarios.

There are two reviews of E3 (energy, economy, environment) models focusing on the transport sector. One [113] reviews 13 models and identifies some key characteristics: elastic demand based on price, endogenous modal choice, choice of no physical travel (avoid demand), demand split by distance (urban and intercity) and infrastructure (to establish a maximum capacity for the transport mode or alternatively investment needed to increase capacity) [113]. The dimension covered by most (11) of the models reviewed was the demand response to price through elasticity, 6 of them had endogenous modal choice, while demand split by distance and infrastructure capacity were covered by only one model respectively. The other one [114] reviews 27 energy and transport models with variable degrees of integration. Behavioral features to be considered in energy and transport systems are: technology choice (also including non-energy cost parameters), modal choice (using travel time budget or constant elasticities of substitution), driving patterns (considering distance and speed) and new mobility trends (e.g. carpooling or autonomous vehicles).

Two previous studies look at FCEV penetration at the EU level. In

b This refers to the linking of a model with explicit consideration of the spatial component or optimization of the hydrogen supply chain.

 $<sup>^{\</sup>rm c}$  GIS approach was used, not for  ${\rm H_2}$  infrastructure, but for spatially locating emissions.

**Table 3** Characterization of modeling approach for JRC-EU-TIMES and PTTMAM.

Model dimension [35]	JRC-EU-TIMES	PTTMAM	Soft-linking consideration
Spatial coverage	EU28	EU28	No adaptation required
Spatial resolution	1 node per country	1 node per country	No adaptation required
Time horizon	2015–2050	2015–2050	Focus on 2050 given that significant FCEV deployment is not expected in the short and medium term
Temporal resolution	12 time slices per year with parametrizations based on hourly data	Annual (delta-time = 0.25)	Annual values taken for commodity prices and powertrain technology mix
Degree of competition	Perfectly competitive	One manufacturer conglomerate <sup>a</sup>	Each model retains its own approach
Demand split <sup>b</sup>	4 (executive, upper and lower medium, small)	3 (small, medium, large)	3 categories are chosen by merging upper and lower medium in JRC-EU-TIMES
Powertrain class	4 (ICEV with different efficiency classes, BEV, hybrid <sup>c</sup> and FCEV)	4 (ICEV, BEV, hybrid and FCEV)	No adaptation required
Energy carriers	10 (gasoline, diesel, CNG, LPG, electricity, gaseous hydrogen, liquid hydrogen, ethanol, synthetic gasoline, synthetic diesel)	8 (gasoline, diesel, CNG, LPG, electricity, gaseous hydrogen, biodiesel, bioethanol)	No liquid hydrogen in PTTMAM. Diesel and gasoline prices from JRC-EU-TIMES already reflect the fuel mix (i.e. include synthetic and biofuels since those are part of the supply curve)
Sectoral coverage	Power, residential, commercial, industrial, transport, agriculture	Transport (cars)	PTTMAM provides a detailed representation of the passenger car transport sector to be used with the other sectors in JRC-EU-TIMES
Mathematical formulation	Linear programming	Differential equations	
Solution method	Single objective (cost) optimization	Euler integration	Each model keeps their own solution method
Purpose	Normative	Explorative	Each model keeps their own purpose
References	[36,116]	[131]	

- <sup>a</sup> Meaning there are no individual manufacturers with different strategies and competition.
- <sup>b</sup> Small = Segment A and B, Lower Medium = Segment C, Upper Medium = Segment D, Executive = Segment E [178].

the deep decarbonization scenario with PRIMES [115], the share of hydrogen in road transport is only 2% with an 84% CO<sub>2</sub> reduction target, while this increases to 31% when the overall CO<sub>2</sub> target is reduced to 96%. This corresponds to a share of 10% of FCEV in the car fleet. A previous assessment with JRC-EU-TIMES has indicated that hydrogen use in transport can be as high as 40 mtpa (4.8 EJ/yr), but where the largest share is actually for heavy-duty trucks and FCEV only represent 10–15% of the car fleet with BEV having a 60% share [36].

In summary, the gaps from literature that are covered in this study are: (1) from the perspective of system dynamics models, the wider scope beyond transport to include interaction with other sectors and how it can affect the total system cost; (2) from the energy system model perspective, it is a step in the direction of improving the behavioral representation characteristic of consumer choices, but where still further work will be needed to consider the potential shift among transport modes and endogenize this behavioral aspect rather than relying on a soft-linking methodology.

#### 3. Modeling approach and structure

This study is based on the soft-linking between two models with EU coverage managed by the Joint Research Centre (JRC): the JRC-EU-TIMES model and the PTTMAM. The reason for this choice is that both models are bottom-up (technology-rich) and have complementary features [51,99]. In this section, each model is briefly described separately, followed by the advantages of combining them and concluded by the parameters that each model uses from each other.

#### 3.1. Description of JRC-EU-TIMES

The model makes the choice for optimal system configuration based on investment, fixed, annual, decommissioning, operational costs and salvage value. It covers EU28 plus Switzerland, Norway and Iceland. To reduce complexity, it uses 12 representative time slices (24 for power sector) to represent a year and it has one node per country [116]. The model generator used is TIMES [117–119]. It combines a normative approach, meaning that the system will reach the pre-established policy

constraints, with an exploratory one, meaning that different future scenarios can be used to understand their impact over the technology mix. It is used by more than 250 institutions in 70 countries [120]. Several policies can be added including  $CO_2$  tax [121], technology subsidy [122,123], regulations, targets, energy efficiency [124], feed-in tariffs, emission trading systems [125] and energy security [126], among others. A common application involves the exploration of decarbonization pathways [84,127–129].

Technologies are represented through their input-output relation, CAPEX, OPEX and lifetime. Individual processes are linked through commodities. Prices are endogenously calculated through supply and demand curves. Some of the key output is the capacity needed for each technology, energy balance for each country in each time period, trading, emissions and total cost. Key assumptions include: perfect foresight (all technology costs, demand for services and balances are known from the beginning of the period), perfect competition (there are no individual players that can influence prices), central optimization (lowest cost decisions made regardless of sectors or borders), no short-term market consideration (e.g. day-ahead, intra-day) and rational behavior. Due to the focus on energy systems (leaving changes in agricultural practices, forestry, other land uses, petrochemical, solvents out of the scope) and only CO<sub>2</sub> (no CH<sub>4</sub>, N<sub>2</sub>O, NO<sub>x</sub> and air pollutants), the model effectively covers around close to 80% of CO<sub>2</sub> emissions.

#### 3.2. Description of PTTMAM

PTTMAM is a simulation model that captures the interactions of the major stakeholders in the light-duty road transport system. Four market agent groups represent these stakeholders: users, manufacturers, infrastructure (refueling and recharging stations) providers and authorities. These market agents are conceptual groupings and not individual agents as in agent-based modeling [130]. Each market agent group follows a set of decision rules that lead to different choices and therefore there is no single objective function. Through a complex interaction between supply and demand time-varying conditions, powertrain choice is determined by the users group. This market agent is influenced by a series of vehicle attributes and a measure of the willingness

<sup>&</sup>lt;sup>c</sup> "Hybrid" refers henceforth to the sum of plug-in hybrid electric vehicles and conventional hybrid ones. In the scenarios analyzed, most (80–90%) of these are PHEV.

to consider a certain powertrain. The former includes financial attractiveness (based on powertrain-specific total cost of ownership), convenience to effective refueling and recharging infrastructure, performance, reliability, environment (i.e. emissions levels) and safety (see Tables 2 and 3 of the model manual [131]). The latter is a modified version of the formulation proposed by Ref. [132], affected by marketing and social exposure. PTTMAM captures the most pertinent EU regulations and initiatives (for a sub-set, see Table SI 2 in Appendix 2). Because of this, the model can be used to conduct policy analysis and explore the impact of certain policy measures on the market uptake of vehicle powertrains.

The model is grounded on the system dynamics modeling approach invented by Jay W. Forrester [133]. This method stresses the importance of relating feedback structure with dynamic behavior and conceptualizes systems as stock-and-flow structures [134]. System dynamics models are based on ordinary differential equations, often solved via Euler numerical integration. The mathematical formulation of PTTMAM leads to over 1500 parameters, out of which 250 are exogenous, and 700000 elements in the model. Heavy-duty vehicles and alternative modes of transport such as rail and buses are not included in the model. PTTMAM has been applied in Refs. [37–39,131,135]. The model was built in Vensim® and is openly accessible through EU Public License [136,137].

#### 3.3. Advantages of soft-linking

A key input for PTTMAM is the prices for energy carriers. In JRC-EU-TIMES prices are the result of the interaction between supply and demand. The supply curve can be changed by introducing new technologies with different raw materials and cost structure, while the demand curve varies when a different energy carrier or end-use technology (e.g. heat pump or gas boiler) is used to satisfy the service. These endogenous prices are also defined by the exogenous import prices assumed for fossil fuels, which are aligned with the EU Reference Scenario [138] and where history has shown that prediction for outlooks is usually poor [139,140] since it can be influenced by sudden fluctuations.

An advantage of using JRC-EU-TIMES as part of the modeling framework is the insight into the competition between sectors for the same commodities. Depending on the scenario, biomass can be more useful in other sectors (even within transport) or hydrogen demand can be mainly defined by a specific application. Similarly, policies affecting the entire system, such as overall  $\rm CO_2$  target, can have different effects depending on the rest of scenario conditions that would be missed if only a target for the transport sector is used. Lastly, alternative supply chains for fuels are also captured and will have an impact on the price of the fuel used by the powertrains (e.g. difference for supplying diesel with Power-to-Liquid or import).

With respect to hydrogen, JRC-EU-TIMES can assess the impact of: (1) different production technologies (e.g. electrolysis vs. biomass gasification); (2) different delivery pathways (there are 20 possible options, see Ref. [36] for associated cost); (3) hydrogen price as a function of electricity price (which in turn is defined by VRE potential and degree of electrification); (4) learning curve for the electrolyzer (which is actually an exogenous parameter, but can be modeled as a sensitivity). These account for elements outside PTTMAM that will be reflected in the hydrogen price. Some of the other elements that are captured better in one of the models and where each one will benefit from soft-linking are captured in Table SI 3 in Appendix 2.

JRC-EU-TIMES deploys powertrains based on CAPEX, OPEX, efficiency and price for the input commodity. In reality, there are more factors determining the choice for powertrains, for example: disposable income per household, average distance per trip, marketing strategies, risk aversion of consumers, popularity and availability of refueling infrastructure, among others. In contrast, powertrain choice in PTTMAM is more elaborate as other factors beyond financial attractiveness are

also considered (see Section 3.2). Furthermore, the role of taxation is explicitly accounted for in this model. In this way, PTTMAM can not only increase the resolution of the dynamics that are usually overlooked in cost optimization, but also complement JRC-EU-TIMES by illustrating that consumer choices are not necessarily based on a purely economic behavioral framework.

Furthermore, economic attributes such as the purchase price and the operating cost of powertrains are shaped by car manufacturers. This aspect of the system, which is absent in the JRC-EU-TIMES model, is covered by PTTMAM. Specifically, supply-side decisions related to pricing and marketing strategies, investment in research and development (R&D) and in vehicle manufacturing capacity are modeled. In PTTMAM, the manufacturers' market agent group reacts to planned EU regulation (e.g.  $\rm CO_2$  target), thereby anticipating the prospect of emission penalties and making business decisions that favor certain powertrains over the rest. As a result, the CAPEX and OPEX evolution for each powertrain vary. Since this remains an exogenous input for JRC-EU-TIMES, incorporating the values of these economic variables from PTTMAM turns out to be desirable.

#### 3.4. Overview of soft-linking process

The purpose of the interaction is to complement the strengths of each model mentioned earlier and by doing so, improve the quality of the resulting policy recommendations. To accomplish this, first, each model needs to be characterized to understand better what the complementary areas and the remaining gaps are. This is presented in Table 3, while the overall framework is shown in Fig. 1.

Two dimensions where the models need to be harmonized are the categories for users and the number of energy carriers. The choice has been made based on simplicity and completeness to leave 3 categories for the former and 8 energy carriers. There is also common input to both that needs to be harmonized to ensure consistency in the output. These are: data for base year (car stock, occupancy, distance traveled), population growth assumption which in turn affects demand, the assumption for the year on which a specific powertrain will become available (2015 for FCEV) and if there is any maximum growth for specific powertrains, to avoid the situation where a particular one attains a large part of the market that might be too drastic or highly optimistic (see Section 4.2).

The other aspect is to understand what variables will be used from one model to the other and how this changes the stand-alone use. This is shown in Fig. 1 along with the basic components of each model.

Fig. 1 only has the choices in the transport sector for JRC-EU-TIMES, while the rest of the system has been omitted. However, relevant input for this module from the rest of the model is the competition of energy carriers among sectors,  $CO_2$  constraint and resulting  $CO_2$  price that will affect the commodity prices, potential for renewable options (solar, wind, geothermal, biomass) that will affect electricity prices and the cost associated to infrastructure development for electricity, gas and hydrogen.

Three approaches to soft-link both models were identified:

- 1. Exclude the choices for powertrain mix in JRC-EU-TIMES and leave the choice and evolution in time to PTTMAM. This can be fed back through fixed shares for each powertrain, country and year that JRC-EU-TIMES will use to determine new supply and demand curves and therefore new commodity prices, new costs to reach the targeted CO<sub>2</sub> constraint, new competition among sectors. The effect of these new prices should be assessed with PTTMAM. For the scenarios analyzed in this study, two iterations were enough to reach stable commodity prices.
- Leave the choices for powertrain mix in JRC-EU-TIMES as part of the optimization process, but instead change the exogenous input to make these choices. This includes CAPEX and OPEX of powertrains by country, size and their (annual) evolution in time, which are an

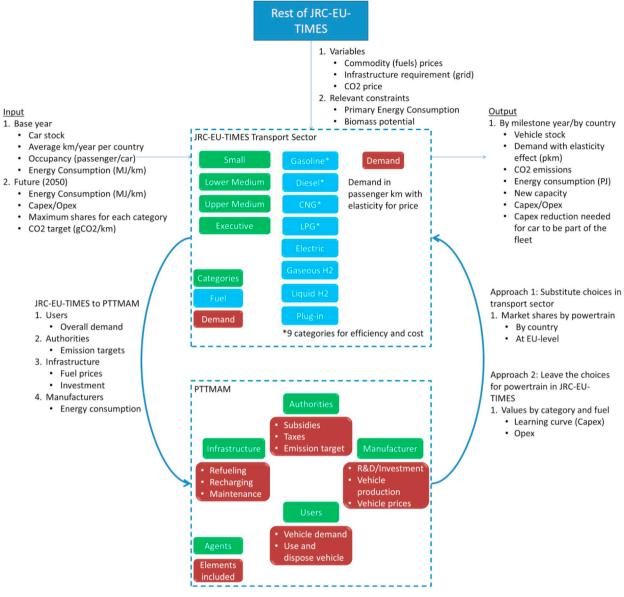


Fig. 1. Soft-linking methodology between JRC-EU-TIMES and PTTMAM.

output of PTTMAM (and therefore scenario dependent). This improves the estimate for the input, while reducing changes in JRC-EU-TIMES, but still makes the powertrain choice purely based on cost. Since this approach would still lead to drastic changes in shares, the constraints from the original JRC-EU-TIMES are kept (see Section 4.2).

3. Change the representation of the transport sector in JRC-EU-TIMES and include additional features such as disaggregated market segmentation to capture different risk adoption profiles, annual driving profile, additional cost for limited spatial distribution of refueling stations, additional cost for cars with limited range and larger disaggregation of vehicle categories for richer choices in powertrains.

For this study, the first two approaches are followed. This allows assessing the difference due to soft-linking methodology, as well as the gap between pure cost optimization and the output from PTTMAM that considers in addition the non-financial aspects. For the first approach, two variations are tested: 1. Specific shares by country and powertrain; 2. Shares at EU level by powertrain (leaving the choice of shares by country to JRC-EU-TIMES).

The third approach to soft-linking, in essence reproducing in JRC-

EU-TIMES the additional calculations performed in PTTMAM, implies larger model changes that need to be validated for a wider range of scenarios. Opting for this modeling approach constitutes one step beyond soft-linking and towards model integration. The incorporation of the features of one model onto the other has already been used in a TIMES model for California [91]. A crucial difference of that model is the scale (a state in a country) in comparison to EU28 covered by the current study.

#### 4. Data and assumptions

#### 4.1. Base year calibration in JRC-EU-TIMES

Part of the exogenous input for JRC-EU-TIMES is the "base year" data, which refers to the start year where all the capacities, energy balance and fuel prices are known and used as starting point for investment choices in the future to satisfy demand for the different services. Specifically for transport, this base year data (see Fig. 1) includes: (1) car stock; (2) mileage per type of car; (3) occupancy rate (different by region) and (4) energy consumption. These parameters are taken from TRACCS database [141] that has enough level of segregation (by

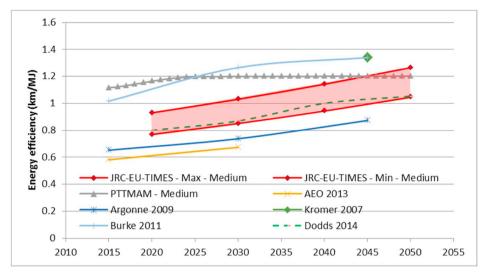


Fig. 2. Energy efficiency for (medium size) FCEV in comparison to previous studies [90,93].

country) and coverage (EU28). To have the same starting point as PTTMAM, the car stock has been updated to match the fuel mix and split by size (small, medium and large) in PTTMAM. The other three parameters (mileage, occupancy rate and energy consumption) have been kept from the original JRC-EU-TIMES data since it is more detailed than what is available in PTTMAM. In particular, mileage (i.e. average annual vehicle-km traveled by car (VKT) or the distance traveled per year) is not differentiated by fuel in PTTMAM. In JRC-EU-TIMES, there are large differences in distance traveled between fuels (diesel and gasoline) based on TRACCS (see Fig. SI 1 in Appendix 3 for data on medium size vehicles). Therefore, those are used for existing vehicles. For new ones the average distance is prorated with car stock and used for all powertrains, assuming cars with similar size will travel the same distance regardless of fuel. In PTTMAM, mileage is an endogenous parameter and this was used to decide if the parameter was soft-linked. Since the average based on car stock in JRC-EU-TIMES was already close to the values used in PTTMAM, no additional change was implemented. There is no further stock or demand split by journey distance.

For calibration in the JRC-EU-TIMES model, the base year is 2010. The main differences in the car stock for the base year were in the split by size and total number of vehicles across EU (see Fig. SI 2 in Appendix 3). The total car stock in JRC-EU-TIMES was originally 240.8 million vehicles [141], while in PTTMAM it was 228.5 million vehicles (6.6% difference). The variation in shares by country was not that significant (see Fig. SI 3 in Appendix 3 for comparison). The other major difference was that JRC-EU-TIMES had almost 10 and 30% more vehicles in the small and large categories, while having 4% lower medium vehicles. The potential effect of this is that the CAPEX differences for powertrains of the same size are different. As an example, BEV might be more attractive than diesel in small cars, but this could be the opposite for large vehicles. Therefore, it will affect the powertrain shares for each size and overall for the total stock since the assumption is that these shares will remain in times (in JRC-EU-TIMES).

#### 4.2. Demand growth for 2050 and exogenous constraints

For subsequent years (until 2050), growth in travel demand by car (total passenger-km (PKM)) has been also aligned with PTTMAM. In JRC-EU-TIMES, total demand of distance traveled is an input to the model. This usually comes from a macro-economic model that takes into account population growth, gross domestic product, employment, among others to estimate such demand. The original demand is aligned with the EU Reference Scenario [138]. In contrast, this parameter is an

output of PTTMAM based on the composition of the car stock. To avoid large differences in output due to this parameter, the demand growth from the baseline scenario for PTTMAM has been used to calibrate the input to JRC-EU-TIMES (see Fig. SI 4 in Appendix 3). For assumptions on hydrogen use in other sectors refer to Ref. [36].

Since JRC-EU-TIMES is based on cost optimization, it will invest in the most attractive (lower cost) powertrain for each period. This could create large swings in car stock [91]. There are additional constraints introduced to prevent this from taking place:

- A range is introduced for the share of new sales of diesel cars within the total sales of fossil cars. A 30% point range is calculated around the average share in 2015, which is calibrated by country based on average diesel shares monitored by the European Environment Agency. This prevents diesel or gasoline being suddenly overtaken by an alternative fossil fuel from one period to the next.
- A minimum of 5% of the 2015 value (in share) for new sales of gasoline vehicles.
- A maximum of 20% of new sales by 2020, 50% by 2040 and it can only reach 100% by 2060 for the total of BEV and PHEV, based on [142].

These constraints are only used in the second approach to soft-linking (see Section 3.4) since the shares come directly from PTTMAM in the first approach. This already introduces a preference for the first approach to soft-linking since it does not require these additional constraints.

#### 4.3. Energy efficiency by powertrain

The FCEV efficiency assumed will have a large influence over its market share since it affects fuel consumption and in turn, the operating cost of the car. In JRC-EU-TIMES this is an exogenous input, which originally came from Ref. [143]. When benchmarking FCEV efficiency in JRC-EU-TIMES with previous studies (collected by Refs. [90,93]), it was found that it lies within the range in literature with similar improvement over time (see Fig. 2). Because of this, it was decided to take the efficiencies from JRC-EU-TIMES as input for PTTMAM. This does not mean that R&D investments are no longer affecting the model results, for those investments still have an impact on other car attributes. However, the variation in time observed in the results was minimal. It is to be noted that in JRC-EU-TIMES, there is an efficiency variation by country and size (based on actual data [141]) for diesel and gasoline vehicles. To avoid promoting FCEV just based on the efficiency

difference for specific countries, the FCEV is varied to keep the same ratio by country (see Fig. SI 5 in Appendix 3 for the range by size). On the other hand, this is an endogenous parameter in PTTMAM influenced by R&D investments. Nevertheless, the improvement in time is limited even in cases where its deployment is significant.

For ICEV, JRC-EU-TIMES has a relation between efficiency (operational  $CO_2$  emissions) and cost [144]. Different than BEV or FCEV, the efficiency improvement in time is not pre-defined, but it is instead an indirect result of the  $CO_2$  target. A lower  $CO_2$  target will trigger more investment in more expensive (and efficient) vehicles increases. Similar than for FCEV, ICEV efficiencies have limited improvement in time and the ones from JRC-EU-TIMES are used as input, assuming that the most efficient vehicles will be deployed by 2050.

#### 4.4. Component cost and price by powertrain

In PTTMAM, the costs of 8 key vehicle components are explicitly modeled. Of particular interest to this study are 3: the fuel cell system, the hydrogen storage tank and the BEV battery. The inclusion of the latter is motivated by the fact that, given strict CO<sub>2</sub> emissions standards for cars that promote the uptake of ZEV, BEV and FCEV enter into direct competition. Component costs are the result of the level of component maturity and the effect of the learning curve in PTTMAM. Whereas the former is influenced by R&D investments (see Appendix 4), the latter depends on the assumed cost reduction fraction associated with learning from cumulative production. Given the future uncertainty of the cost evolution of these components, sensitivity analyses on the assumed learning rate (by default 10% for each component, except for the ICE which is 1%) were conducted. Based on Monte Carlo simulation (200 runs using a uniform probability distribution) performed in PTTMAM on the three components, the BEV battery cost was identified as the most influential variable. In Fig. 3a, the BEV battery price resulting from learning rates of 5% (low - dashed curve) and 15% (high dotted curve) can be seen (see also Fig. SI 8 in Appendix 3).

Fig. 3 also shows the price evolution of these three components in PTTMAM, compared with information from various sources (for the EV battery, refer also to Fig. 5.1 in Ref. [149]). The price of components was derived using a default mark-up of 10% over the costs (also applied to values from literature whenever it was interpreted they were referring to cost). With regards to the simulated price evolution of the BEV battery (Fig. 3a), it is higher than the historical data until 2018 and the values projected by Ref. [19]. The price in 2030 is, however, within the values available in the literature. By 2040, a value of 57 €/kWh was simulated, which falls to 52 €/kWh by 2050. With respect to the FCEV components (Fig. 3b), both the fuel cell and the hydrogen tank have a steep price decrease until 2030 with almost a flat trend after 2030. Compared to literature, the initial price values found by the Hydrogen Council [21,148], based on low volumes, are lower than the ones from PTTMAM. Particularly ambitious seems to be the 2020 target value of 33 €/kW (page 69 [148]), given the purchase price of FCEV currently available in the market and the limited number of models expected to be launched in the near future. In 2040, PTTMAM simulates a price of 14 €/kW for the fuel cell. It is assumed that the medium BEV has a battery size of 30 kWh and the medium FCEV features a 90 kW fuel cell system and a 4.8 kg storage tank. Fig. 3b shows that faster price reductions in the two main FCEV components occur in the *Ambitious H*<sub>2</sub> scenario than in the *No CCS* scenario (see Section 5).

In PTTMAM, R&D investments by manufacturers are influenced by the possibility of incurring in  $CO_2$  emission penalties. Strict  $CO_2$  emission targets can be expected to divert R&D investment towards ZEV. Overall, the cost simulations in PTTMAM reflect the anticipation of manufacturers to the prospect of more stringent  $CO_2$  targets, which eventually lead to faster cost reductions for the three powertrain components and subsequent fluctuations in cost reduction from one year to the next (as shown in Fig. 3). This introduces a more realistic cost curve that is not completely smooth, while also carrying an uncertainty associated to the relation between  $CO_2$  target, long-term profit expectation by powertrain and fraction of R&D invested.

#### 5. Scenario definition

The scenarios approach used is technical, in the sense that they do not rely on storylines [150–152]. This means that key input parameters are changed to analyze their effect rather than relating them into plausible dynamics to depict alternative futures. This analysis was already done with JRC-EU-TIMES [36] and the three parameters that have the most influence on hydrogen deployment (other parameters in Table SI 3 in Appendix 2) are:

- CO<sub>2</sub> target. 95% CO<sub>2</sub> reduction by 2050 (vs. 1990) could increase hydrogen flows by 50–80% compared to an 80% CO<sub>2</sub> reduction target. This CO<sub>2</sub> target is for the entire energy system, whereas the reduction by sector (e.g. passenger transport) is a result of the cost optimization.
- CO<sub>2</sub> underground storage. This option could be limited due to social
  acceptance or political interests. In such case, it excludes gas steam
  reforming as hydrogen production technology, requiring a larger
  electrolysis capacity. At the same time, limiting the technology
  portfolio, demands more from the options left (including hydrogen)
  in order to achieve the CO<sub>2</sub> target.
- Biomass potential. Biomass can be used across all sectors (including hydrogen production) and can provide neutral CO<sub>2</sub> for electrofuels downstream (if sustainability criteria is established and respected), so it provides CO<sub>2</sub>-free energy. Ranges explored for EU28 are 7–25.5 EJ/yr [36].

In PTTMAM, the assumption on further evolution of the  $\rm CO_2$  emission regulation for cars is crucial for the market penetration of FCEV. Without a strict  $\rm CO_2$  target for the EU28 average new car sold, the uptake of this powertrain is minimal (as already analyzed in Ref.

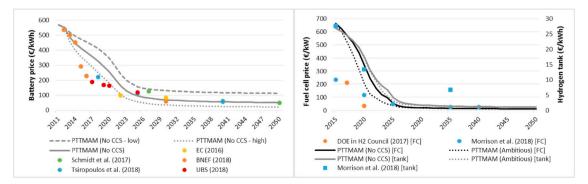


Fig. 3. Price evolution of key powertrain components: (a) BEV battery; (b) FCEV. Source: data/projections shown in the legend and own simulations [19–21,145–148].

**Table 4**Parameter combination for main scenarios.

	JRC-EU-TIMES		PTTMAM				Soft-linking	
Scenario Low Carbon	CO <sub>2</sub> target -95%	CO <sub>2</sub> storage Y	Refueling station N	Purchase subsidy N	Vehicle discount N	Fuel subsidy N	R&D subsidy N	Approach 1 and 2
No CCS	- 95%	N	N	N	N	N	N	Approach 1
Ambitious H <sub>2</sub>	<b>-95</b> %	N	Y	Y	Y	Y	Y	From JRC-EU-TIMES to PTTMAM

#### [135]).

These parameters and policy instruments are combined in 3 main scenarios with the rationale explained below and with the choice for parameters shown in Table 4.

- Low Carbon. It has 95% CO<sub>2</sub> reduction for JRC-EU-TIMES, possibility of CO<sub>2</sub> underground storage and a biomass potential of 10 EJ/yr.
- No CCS. CO<sub>2</sub> underground storage has a large impact in CO<sub>2</sub> prices and technologies chosen. At the same time, it faces social acceptance issues and it has a large impact on technology choices. The only difference of this scenario compared to *Low Carbon* is the absence of CO<sub>2</sub> storage.
- Ambitious H<sub>2</sub>. Under this scenario, which is derived from the *No CCS* scenario, a pro-FCEV policy package comprising the 5 policy instruments (see Table 5) is simulated.

The Low Carbon scenario has already been explored in detail with JRC-EU-TIMES [36], but it represents a new space explored for PTTMAM, where the *Baseline* scenario from Ref. [131] had much higher  $\rm CO_2$  emissions (84 gCO<sub>2</sub>/km for 2050 vs. 5.2 gCO<sub>2</sub>/km in the *Low Carbon*). The comparison of this previous scenario from PTTMAM with the Low Carbon scenario in this study is discussed in Fig. SI 9 and 10 of Appendix 5.

#### 5.1. Policy instruments explored for FCEV

In addition to the system-wide parameters considered above, there are also technology-specific policy instruments that are relevant for hydrogen, especially to kick-off deployment and the learning process needed for cost reduction. The range of policies that can be used for low-carbon transport is covered in Table SI 2 in Appendix 1, including its coverage by JRC-EU-TIMES and PTTMAM. The ones selected for this study (used for the *Ambitious H*<sub>2</sub> scenario) are:

- FCEV purchase subsidy (or tax exemption) by authorities. The same
  way it has been applied for BEV [153], reducing the cost penalty for
  the consumer could increase attractiveness, uptake and minimum
  deployment level to reduce cost (besides wider set of choices for the
  consumer and an optimized manufacturing process).
- Vehicle discount by manufacturers. In theory, this could happen if car manufacturers forecast that they will have to pay emission penalties unless they sell more ZEV. It can also be considered to be a marketing tool.
- Fuel subsidy (or tax exemption). Currently CAPEX for electrolyzers is still relatively high (1200–1500 €/kW for PEM) and it could lead to high hydrogen prices without taxes (depending on operating

hours and average electricity price paid) of  $6-8 \text{ } \ell/\text{kg}$  [154]. This subsidy is also equivalent to financing of the rest of hydrogen infrastructure (e.g. pipelines, delivery trucks, compression).

- H<sub>2</sub> refueling station investment. Governments could financially support in an initial development to reduce risk for investors and provide certainty for investment. Infrastructure availability affects the convenience attribute and consequently the car choices made by the users.
- R&D subsidy (see Appendix 4). This would tackle the "learning-by-research" component rather than "learning-by-doing", with the same common target of reducing the CAPEX. The two most expensive components of FCEV are the fuel cell and the hydrogen tank. R&D subsidy is tested for the fuel cell only and for both components. This considers the relation between R&D subsidy and potential cost decrease, but it is not technology explicit (e.g. consider a different technology for storing hydrogen). This subsidy is triggered by the *Authorities* agent of PTTMAM.

This list of instruments does not cover all the possibilities for policy-making. Other financial incentives with the potential to influence powertrain choice are vehicle tax (exemptions) such as registration, circulation and value-added taxes [155]. Even though technology specific policies can result in a higher cost for society [156], there are cases (e.g. R&D) where it is attractive [157]. Technology-specific policies are also favored to bridge the gap between invention and large scale diffusion and that have potential to reduce cost by economies of scale [157] making possible a lower life cycle cost in the long term [158].

#### 5.2. Sensitivities on policy instruments for FCEV

Table 5 shows the assumed timing and numerical values for the 5 aforementioned policy measures. The individual effect is explored in the results and when simulated together, they represent the pro-FCEV policy package under the Ambitious  $H_2$  scenario. A numerical value of 100% for hydrogen infrastructure investment means that the cost of building a H2 station for infrastructure providers becomes fully subsidized by the authorities over the period 2030-2034. The proportion of FCEV subsidy, equal to 25%, translates into government subsidies that range from approximately 8-11 k€ in 2020 to 0.3-1.5 k€ for small FCEV in 2024 (for medium and large FCEV, the price differential reaches zero by then). For comparison, rebates amounting to 4-6 k€ are offered for FCEV in California [159]. Concerning fuel subsidies, the assumed value leads to H2 pump prices that are on average 60% lower than without subsidies. The R&D subsidy refers to expenditure in improving the fuel cell system. For reasons of simplicity, changes in subsidies have been implemented in the model runs as step changes and not gradual

Table 5 Pro-FCEV policy measures under the *Ambitious*  $H_2$  scenario.

Policy instrument	PTTMAM parameter	Period for subsidy	Subsidy
Purchase subsidy as vehicle discount	Manufacturer vehicle subsidy	2030–2034	5 k€/car
Purchase subsidy	Authorities vehicle subsidy proportion <sup>a</sup>	2020-2024	25%
H <sub>2</sub> refueling station investment	Authorities desired infrastructure support	2030-2034	100%
Fuel subsidy	Authorities fuel subsidy	2030-2034	100%
R&D subsidy	Authorities subsidy for R&D expenditure	2020–2024	5 bln€

<sup>&</sup>lt;sup>a</sup> Of price differential between the FCEV and the gasoline car.

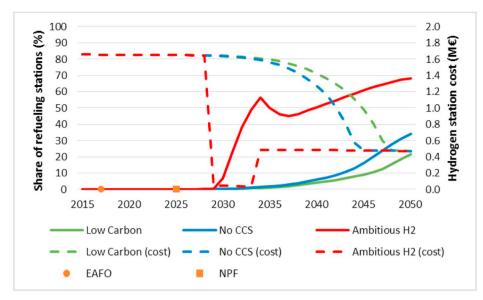


Fig. 4. Share of H<sub>2</sub> refueling stations in the EU28 [28,160], by scenario, and cost of deployment (right).

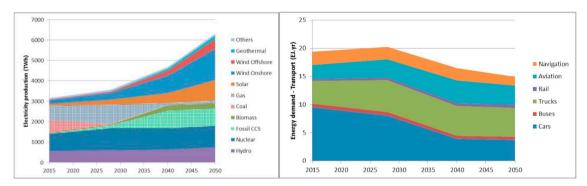


Fig. 5. (a) Electricity mix (b) Energy demand for transport in the Low Carbon scenario.

changes. This means for example, the subsidy for refueling stations in 2029 and 2035 is zero, as compared to 100% during the 2030–2034 period. These policies are implemented for all Member States.

Concerning H<sub>2</sub> refueling infrastructure, due to these subsidies in the Ambitious H2 scenario and subsequent economies of scale, the simulated cost of a H<sub>2</sub> station decreases from 1.6 M€ in 2030 to 0.5 M€ after the policy period. Fig. 4 shows how H<sub>2</sub> station deployment and cost varies by scenario (endogenous in PTTMAM). Whereas the European Alternative Fuels Observatory (EAFO) data point [28] is based on 82 H<sub>2</sub> stations, the National Policy Framework (NPF) point is the result of summing up the 2025 values communicated by the Member States in the context of the Directive 2014/94/EU [160]. In all the scenarios, the total number of refueling stations in the EU28 is 118000, as simulated in PTTMAM. As can be seen, H2 refueling availability is wider in the Ambitious H2 scenario than in the Low Carbon and No CCS scenarios, facilitated by the drastic decrease in the cost that infrastructure providers face due to the subsidy. The impact of infrastructure investment over the 2030-2034 period leads to achieving the minimum cost of 0.5 M€ earlier than the other scenarios and a maximum coverage of H<sub>2</sub> refueling stations of 70%. However, the simulation shows that this market is not yet self-sustained and there is a slight decrease in H<sub>2</sub> refueling availability once financial support is removed in 2034 and infrastructure providers need to pay the investment.

#### 6. Results and discussion

Results are divided in three sections: (1) transport in context of the energy system (Section 6.1) (2) soft-linking process, how it affects the

stand-alone output of each model and the impact it has on the rest of the energy system (i.e. total cost and hydrogen prices) (Sections 6.2 and 6.3); (3) FCEV deployment to identify drivers, most effective policies and the level of investment or subsidies needed (Section 6.4). To facilitate understanding, each section starts with the two most important ideas followed by the more in-depth explanation and each paragraph starts with a header with the main topic discussed.

## 6.1. Overview of the transport sector and relation with the rest of the energy system

BEV and FCEV can increase electricity demand by around 600 TWh at a similar cost than a high  $\rm CO_2$  scenario and a benefit of 60% reduction in energy consumed. PtL can be attractive for cars in a world with high biomass potential and no CCS.

The  $CO_2$  footprint of ZEV is largely defined by the upstream production of the fuel (different from current ICEV where most of the emissions are upon end-use combustion). The electricity mix for the Low Carbon scenario is shown in Fig. 5a. At the same time, it is expected that the higher ZEV efficiency leads to lower energy consumption and the share from passenger transport is put in context of the total transport energy demand (Fig. 5b).

**Electricity production.** Electricity production grows from almost 3200 TWh in 2015–6300 TWh by 2050. The largest contributors to this growth (see Fig. SI 20 in Appendix 6) are the electrification of heating in the residential and commercial sectors (+750–850 TWh), hydrogen production (+700–800 TWh) and industry (600–650 TWh). This scenario still has CCS as a possibility, resulting in gas reforming as main

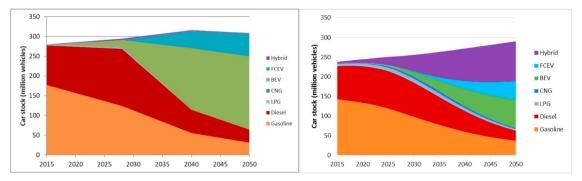


Fig. 6. EU28 powertrain mix from (a) JRC-EU-TIMES before soft-linking; (b) PTTMAM (equivalent to the "after soft-linking" since the shares are an input to JRC-EU-TIMES in this approach) for the Low Carbon scenario.

production route (see Section 6.1). In case CCS is not possible, combined with the efficiency loss for electricity to hydrogen conversion, the total electricity demand increases to almost 10000 TWh (3× current system) and almost 1000 GW of electrolyzers are needed. To be able to achieve a low electricity footprint and reach the desired benefit in downstream sectors, fossil fuels are phased out. Coal is phased out by 2025-2030 and most of gas by 2040. These are partially replaced by gas in combination with CCS to be able to provide flexibility to the power system, while still restricting the CO2 emissions. Nuclear and hydro remain mostly at the current level, considering that further expansion of the nuclear capacity in some countries is combined with nuclear phase-outs in other countries. These conventional sources have a similar production level (2800 TWh) than in 2015. Most of the growth is supplied by VRE that reach almost 3300 TWh by 2050. This in turn translates into almost 1000 GW of solar and 850 GW of wind needed by 2050.

Transport energy demand. Due to electrification of the passenger transport, its energy demand decreases from almost 10 EJ/yr in 2015 to 3.8 EJ/yr by 2050. Heavy-duty trucks instead increase their demand 40% by 2050 (vs. 2015). They shift mostly to hydrogen and the higher efficiency (compared to ICE) compensates the higher ton-km demand keeping the overall energy demand increase to only 27%. With these changes, the share of energy demand from passenger transport halves from 56% in 2015 to 28% in 2050. This also translates into a smaller increase in the electricity demand of 550 TWh.

System cost breakdown. The total (sum of CAPEX, OPEX and fuel for all powertrains) cost contribution of the passenger transport sector is 800 bln€/yr for the *Low Carbon* scenario. The split is close to 65/35 in CAPEX/OPEX. To put this in perspective, the cost of the overall road transport sector (including heavy-duty trucks and buses) is almost 1700 bln€/yr by 2050 [36], while the total energy system costs (including other sectors) is 3500–4000 bln€/yr. Already by 2030, the cost differential between ZEV and ICEV has closed considering the learning effect for the former and the higher CAPEX due to efficiency improvements for ICEV.

Higher biomass potential. Using a higher biomass potential (25.5 EJ/yr [161]) in the *Low Carbon* scenario increases the number of gasoline and diesel vehicles in 2050 compared to the scenario with the reference biomass potential, increasing their share from 7% of the fleet to almost 34%. This growth does take some share away from FCEV, which decrease to 4.3% of the car fleet. This increase in ICE is not the direct product of more biofuels due to the higher biomass potential. Instead, more biomass is coupled with CCS, which allows negative emissions and enables positive emissions from the use of fossil fuels in transport. Fossil fuels go from 0.4 EJ/yr with a reference biomass potential to 3.5 EJ/yr with a high biomass potential (see Fig. SI 14 in Appendix 5). This is still lower than the 12 EJ/yr of the base year. Biofuels for cars increase from 0.75 EJ/yr to 2.2 EJ/yr. Without CCS, there is no possibility of offsetting the positive emissions from transport and even in this scenario, ICE reach around a third of the car stock.

However, the largest change in the fuel mix is from a higher supply from PtL that uses the biogenic  $\rm CO_2$  and nearly triples its production to reach almost 60% of the diesel supply, while biofuels (mainly through BtL) supply the balance of demand. Therefore, even with a high potential biomass plays a limited role directly in passenger transport. With a reference potential of  $10\,\rm EJ/yr$ , biomass is better used in sectors like aviation, maritime transport and heavy-duty [36].

For more details on the outlook of the wider energy system and changes due to low carbon scenarios as well as sensitivities, refer to Ref. [36].

#### 6.2. Soft linking – approach 1 – powertrain shares

Considering the behavioral aspects in passenger car transport changes the solution from the cost optimal resulting in 14% higher total cost for this sector. During early stages of deployment, using hydrogen from gas reforming for FCEV can be attractive.

FCEV shares. For both soft-linking approaches, a stricter CO<sub>2</sub> target was introduced in PTTMAM that was taken from JRC-EU-TIMES results (5.2 gCO<sub>2</sub>/km). The fleet is dominated by hybrid vehicles (30%) followed by BEV (24.5%), ICE (24%) and FCEV (16.5%) (see Fig. 6b). This allows achieving 16.7 gCO<sub>2</sub>/km for the new vehicles. This is better than the 84 gCO<sub>2</sub>/km PTTMAM had as starting point, but still not low enough to achieve the target set by JRC-EU-TIMES (which has a higher BEV share as shown in Fig. 6a). To put this in perspective, in a scenario with PRIMES looking at 80% CO<sub>2</sub> reduction (for the entire system) with faster learning curve for fuel cells and a CO2 standard of 16-23 gCO2/ km, FCEV achieve 16% of the car stock by 2050, BEV have the largest (51%) share and hybrids are 17% [162]. When targeting a net-zero emissions pathway, which translates into 90% GHG reduction for transport and 0 gCO<sub>2</sub>/km for new vehicles from 2040 onwards, FCEV remain at a similar level (16%), while BEV increase their share to 80%. Nevertheless, no combination of a net-zero emissions pathway and a high learning rate for fuel cells was considered in Ref. [162]. Another study with PRIMES [163] looking at a scenario where the decarbonization strategy fails to develop during the 2020-2030 decade. This translates into higher emissions during this decade that are compensated later on with a CO<sub>2</sub> target of 5 gCO<sub>2</sub>/km in 2050 to stay within the 155.5 GtCO<sub>2</sub> of cumulative emissions until 2050. With this stricter target, the fleet has 7% FCEV and 78% BEV in 2050 (where the latter grows from 27% of the car stock in 2040). The Hydrogen Council has 400 million FCEV on a global basis as part of their 2050 vision [148], which would imply a larger FCEV stock in EU than the 48 million FCEV obtained in the present study.

In the first approach, the choices for powertrain mix are excluded from JRC-EU-TIMES. The car stock shares were fed back from PTTMAM to JRC-EU-TIMES in two modes: (1) Country specific for four milestone years (every 10 years from 2020 to 2050); (2) Overall EU shares (leaving the degree of freedom in JRC-EU-TIMES to allocate shares to specific countries). Fig. 7a shows the country specific shares obtained

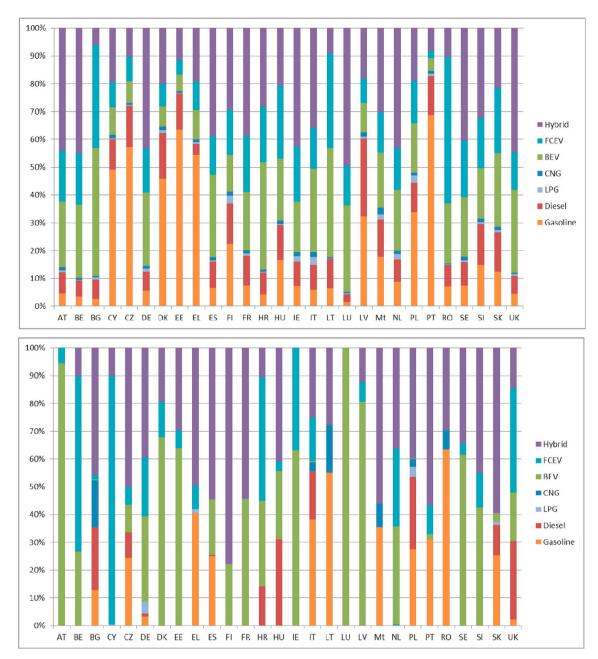


Fig. 7. Country specific powertrain shares for the Low Carbon scenario in 2050 (a) Shares from PTTMAM (b) Optimized shares when using shares at EU level.

from PTTMAM. In one scenario these shares are exactly achieved by JRC-EU-TIMES since it is used as constraint. However, this leads to a more constrained system.

Country vs. EU shares – Hydrogen prices. When only using the overall EU share as constraint, it can be seen (Fig. 7b) that it is better to exploit the countries with low electricity and hydrogen prices to increase the BEV and FCEV shares in those countries, while leaving gasoline and diesel vehicles for the countries with higher prices (noting that gasoline and diesel prices are almost the same across countries since taxes are not included). This is also the case for the *No CCS* scenario (see Fig. SI 15 in Appendix 5). This enables lower hydrogen prices, since countries with expensive hydrogen do not need to use it anymore and on average hydrogen is 0.4 €/kg cheaper when taking the EU shares, but the benefit can be as high as 2.2 €/kg for Sweden (see Fig. SI 11 in Appendix 5). Differences for the two scenarios can be explained based on: 1. The technology mix for hydrogen production; 2. Distribution route for hydrogen and 3. Magnitude of hydrogen demand

for FCEV compared to the total demand. For example, for Sweden, hydrogen is mainly produced by biomass gasification when the hydrogen demand is the lowest (i.e. EU shares – Fig. 7b). However, when the hydrogen demand is forced to be higher (by specifying the FCEV share), the marginal contribution is by gas reforming with CCS and a more expensive distribution route (smaller refueling stations that have a more pronounced effect than production technology) leading (mainly the latter) to a higher hydrogen price.

Country vs. EU shares –  $CO_2$ . Similar to the large fluctuations in powertrain mix by country when the shares at EU level are used, there are large differences in  $CO_2$  emissions for the car fleet depending on the approach used (see Fig. SI 12 in Appendix 5). For example, Denmark has an average  $CO_2$  emission for the fleet of 43.4  $gCO_2$ /km when the country specific shares are used, but only 9.1  $gCO_2$ /km when the overall EU shares are used (in 2040). Exploiting the wind potential in Denmark leads to lower electricity prices and to increase the BEV share beyond the output from PTTMAM leading to lower average emissions

from the fleet. Similar cases occur in Finland, Austria and Ireland.

Country vs. EU shares - Total cost. In spite of these large changes in composition, when looking at the total cost for passenger transport including CAPEX, OPEX and fuel cost, the differences are smaller (see Table SI 5 in Appendix 5 for the cost breakdown). The cost is only 0.5% lower for the entire period when shares at EU level are considered (compared to country shares) with a larger difference (1.2% lower annual cost for EU shares vs. country shares) for 2050. When the boundaries are expanded to cover the entire energy system, cost differences for the additional flexibility translate into a marginal CO<sub>2</sub> price increase of 20 €/ton. This is an indication that there are alternative pathways with very similar cost (i.e. near optimal), but with large differences in technology mix. This is a well-known characteristic of energy cost optimization models [168], where other factors such as energy security, exposure to high commodity prices [169], risk [170], societal aspects [171], sustainability [172], among others should be considered to select the best set of policies and pathway to achieve the low-carbon future.

**Soft-linking effect – Cost.** When comparing the costs for the *Low Carbon* scenario before and after fixing the shares from PTTMAM (see Fig. SI 13 in Appendix 5), there is a 14% increase in the total (CAPEX, OPEX and fuel) costs for passenger vehicles. This means adding the extra attributes that PTTMAM covers (e.g. performance, reliability and convenience), deviates the solution from the cost optimal. Therefore, feeding back the shares from PTTMAM does cause a large difference in both cost and powertrain mix. The limited impact is on how these shares are fed back (country specific vs. EU level).

**Hydrogen production pathways.** The hydrogen price was found to actually increase in time instead of decreasing along with the cost curve for electrolyzers (see Fig. SI 16 in Appendix 5). For the first few years when FCEV are starting to enter the market, it results better to use relatively cheap hydrogen from steam reforming (starting at 1.5 €/kg). This allows compensating a high CAPEX for the vehicles with a low OPEX (decreasing the need for subsidy) and it still results in lower wellto-wheel CO2 emissions than ICEV [164-166]. At the same time, hydrogen flows in these early years (before 2030) are relatively small (1%) of the full demand in 2050, decreasing the possibility of a lock-in effect. By 2030, the CO2 target becomes more stringent leading to higher CO2 prices, while hydrogen is also being used for other sectors increasing the demand. Both of these effects lead to higher hydrogen prices (2.5-5 €/kg). The higher CO<sub>2</sub> price also leads to reforming becoming less attractive due to the higher penalty associated to the remaining emissions after capture. In parallel, CAPEX for electrolysis is lower and there is more wind and solar capacity leading to lower cost electricity and need for flexibility. Therefore, after 2030, when hydrogen flows start to increase substantially, most of the growth (> 98%) is in electrolysis (complemented by biomass gasification). The factor with the largest influence on hydrogen production (and electrolysis) is the use of CO2 storage (see Fig. 8 and [36]). With CCS available (Low Carbon scenario), gas is used as dominant technology and electrolysis is deployed 10 years later to a smaller extent. The effect on hydrogen prices is that without CCS, there are fewer options to achieve the  $CO_2$  target, leading to higher  $CO_2$  prices and therefore higher hydrogen prices (by  $\sim 1~\text{€/kg}$ ). To put these numbers in perspective [47], estimated a hydrogen cost of 4.35~€/kg (including wind turbines, electrolyzer, storage and transmission) for a hydrogen-tomobility scenario in Germany [80], estimated a production cost at the refueling station of 3-6.4~€/kg considering the cost uncertainty for each step in the production chain and [167] estimated between 6.5 and 8 €/kg including electricity, hydrogen production, storage and refueling considering an electrolyzer cost of 720 €/kW and a corresponding efficiency of 70%.

#### 6.3. Soft linking - approach 2 - CAPEX and OPEX

Only using the costs from the simulation model has the disadvantage of not capturing fully the behavioral aspects rendering this approach less attractive than using the powertrain shares directly. Also, when non-disruptive scenarios are not desirable, still additional constraints are needed in the cost optimization model.

This approach evaluates the difference in powertrain mix when using JRC-EU-TIMES, but with the CAPEX and OPEX updated from PTTMAM. The comparison between the original CAPEX for ZEV (continuous lines) and the ones from the *Low Carbon* scenario in PTTMAM (dashed lines) are shown in Fig. 9. The reason to focus on ZEV is that these are key options to achieve so low CO<sub>2</sub> targets (< 10 gCO<sub>2</sub>/km for the average fleet) in 2050. Originally in JRC-EU-TIMES there was no differentiation of CAPEX by size because the shares by size were fixed throughout the entire period and there was no possibility of changing demand from one size to the other. This leads to only two lines presented in Fig. 9 for the original JRC-EU-TIMES. In contrast, the CAPEX used from PTTMAM does have the differentiation by size and considering the evolving fraction for each size.

FCEV Capex differences. The CAPEX for all the FCEV sizes is below the one from JRC-EU-TIMES beyond 2026 with a difference of almost 4 k€ for the small vehicles in 2050. At the same time, the CAPEX for BEV from PTTMAM is higher than the original one in JRC-EU-TIMES. Given that the *Low Carbon* scenario already had almost a 16% FCEV share in the car stock by 2050, it is expected that these more optimistic CAPEX for FCEV will only increase this share, unless the higher share, which results in higher hydrogen demand increases the price enough to make FCEV too expensive (in terms of total cost of ownership) in spite of the lower CAPEX. However, this is not the case and FCEV dominate due to the lower CAPEX (see Fig. 10).

**Powertrain shares.** When taking the updated cost from PTTMAM and leaving the choice to JRC-EU-TIMES with no constraints, it chooses FCEV from 2040 onwards when the  $\rm CO_2$  target is strict enough to require low emissions from this sector and given that it is more attractive than BEV, it becomes the dominant powertrain (Fig. 10a). Since this drastic change based on pure cost optimization is optimistic, that is why the additional constraints on diesel, gasoline, CNG, LPG and BEV were added in the first place (see Section 4.2). Only when the original

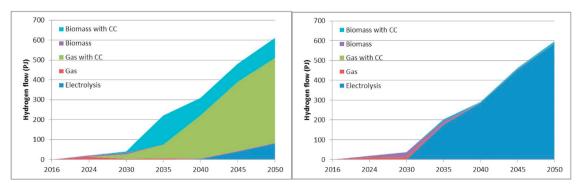


Fig. 8. Hydrogen production mix for passenger transport in (a) Low Carbon and (b) No CCS scenarios.

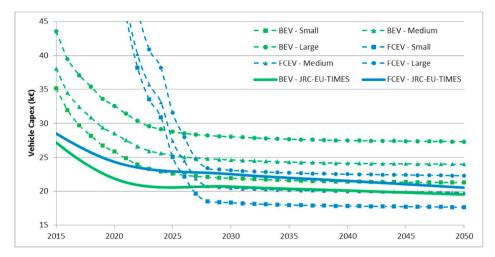


Fig. 9. CAPEX comparison for BEV and FCEV between original values in JRC-EU-TIMES and output from PTTMAM for the Low Carbon scenario.

additional constraints are added, the transition has less abrupt changes (Fig. 10b). However, in the competition among ZEV, FCEV still dominate. The lower FCEV CAPEX outweighs the higher pathway efficiency for BEV. Even though these constraints can be seen as artificial (and will differ by specific TIMES model), they do avoid highly disruptive or highly ambitious changes (FCEV go from 0% of the car stock in 2030 to 93.3% 10 years later) in the car stock. The use of this approach does result in 12% lower transport cost (see Fig. SI 13 in Appendix 5) since FCEV is the dominant powertrain and the soft-linked CAPEX is lower than originally in JRC-EU-TIMES (Fig. 9). As soon as the additional constraints are added, the total cost increases by 20% reaching the same level as Approach 1 (with country shares).

When comparing this Approach 2 (i.e. updating CAPEX and OPEX plus additional constraints) to Approach 1 (directly use the shares), Approach 1 has the clear advantages of: (1) avoiding additional constraints that might be arguable or ad-hoc; (2) considering other aspects besides cost and it is the preferred method to soft-link it both models.

#### 6.4. Policies effect on FCEV deployment

Combining R&D investment in 2020 with infrastructure, purchase and fuel subsidy in 2030 is the most effective policy mix to promote FCEV deployment.

This section shows the market share for FCEV for different scenarios (see Section 5.2). Support policies are implemented individually to evaluate their effectiveness in 3 different periods. The effectiveness is measured through cumulative number of sales over the entire period (2015–2050) since (1) the timing for each one is different and (2) they can have an effect after the policy has been removed. All the policies have been evaluated in the *No CCS* scenario (assuming the reference learning rate of 10% for FCEV) and the policies with the largest impact

are combined in the *Ambitious H\_2* scenario. This scenario includes softlinking from JRC-EU-TIMES to PTTMAM, but feeds back neither the shares nor the CAPEX and OPEX to JRC-EU-TIMES and it is only meant to assess the effectiveness of the various policies in FCEV diffusion. The individual and combined effects are shown in Table 6 and Fig. 11.

**Policy effectiveness.** The effect of each instrument on cumulative (2015–2050) FCEV sales is shown in Table 6. The *No CCS* scenario (without any FCEV policy) has cumulative sales of 67 million vehicles. The main insights are:

- The measure with the largest <u>net</u> impact is the 5 k€ vehicle discount over 2030–2034, which reaches 24.3 additional million FCEV for a total incentive of 84 bln€. The largest impact occurs when it is introduced in the latter period, where the 5k€ represents 22–28% of the FCEV CAPEX (depending on the size).
- The policy with the highest <u>specific</u> impact is R&D, where the FCEV sales increase is 2.1 million for every bln€, while it is only 0.28 million FCEV for every bln€ spent as purchase subsidy (from manufacturers)
- Infrastructure and fuel subsidy have the lowest specific impact at 0.12 additional million FCEV for every bln€ spent (113 bln€, most of which goes to infrastructure development).
- R&D investment is more effective when used for the fuel cell system
  rather than equally split between the fuel cell and the tank. The
  effect of the same 5 bln€ results in 10.5 additional million FCEV
  when invested in fuel cell, while only 5.6 additional million FCEV
  when equally split in both components.
- Contrary to expectations, delaying the infrastructure support to 2030 has a beneficial effect on sales resulting in 14 additional million FCEV when introduced in 2030 compared to only 0.3 additional million FCEV when introduced in 2020. This is because in early

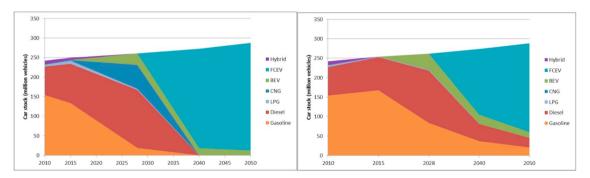


Fig. 10. EU28 powertrain mix for the Low Carbon scenario from JRC-EU-TIMES (a) Only updating CAPEX and OPEX from PTTMAM (b) Updating CAPEX and OPEX plus adding original constraints.

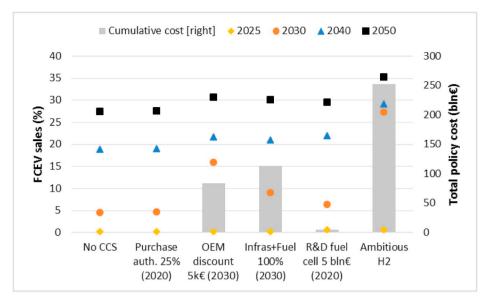


Fig. 11. EU28 FCEV market share by policy scenario (left axis) and cumulative cost (right).

periods there is limited infrastructure deployment that takes advantage of the subsidy, while later deployment results in a higher total subsidy.

Policy mix. R&D expenditure is more effective in 2020, while infrastructure, fuel and purchase subsidies are more effective in 2030. These are combined in the Ambitious  $H_2$  scenario, which reaches an additional 56.5 million FCEV of cumulative sales for a total incentive of 252 bln€. There is a synergistic effect between policies and the increase in total number of sales from the Ambitious  $H_2$  scenario is larger than the sum of sales for each individual policy. This comes however, at a higher cost of 252 bln€, which actually means a lower effectiveness of incentive at 0.22 additional million FCEV for every bln€ spent. If the policy target is to promote FCEV deployment, the combination from the Ambitious  $H_2$  is the most attractive since it comes at a similar marginal benefit for the incentive. Part of the benefit not reflected in Fig. 11 is that this extra cost is partially offset by the lower CO2 emission penalties that manufacturers would face in the Ambitious H2 (vs. No CCS scenario). When looking at FCEV sales (Fig. 11), the Ambitious H2 scenario reaches more than 25% already in 2030, staying at a similar level in 2040 and increasing slightly until 2050.

Comparison with previous studies. To put some of these numbers in perspective [159], claims that the cost to construct 60 HRS in 2017 was 167 M€ and the Hydrogen Council [148] indicates that around 17 bln€ are needed to build an HRS network of 15000 stations. In 2008, it was estimated by the HyWays project that an HRS network between 13000 and 20000 HRS would cost around 15 bln€ [173]. McKinsey estimated a cost of 54 bln€ for the hydrogen distribution and retail

infrastructure for a 25% (68 million) FCEV penetration in EU by 2050, while this cost would rise by another 75 bln€ for 50% FCEV penetration [174]. In Germany, the total (production, distribution and refueling) infrastructure cost for an FCEV fleet of 20 million was estimated at 20 bln€ [175]. The same study [175] has an overview of the infrastructure for previous studies including 100 bln€ (total infrastructure cost) for a fleet of 42–45 million. In terms of R&D, the European automotive industry invests around 54 bln€ in R&D each year [176].

Ambitious H<sub>2</sub> scenario. In Fig. 12a, the evolution of the FCEV sales and stock in the EU28 between 2015 and 2050 on an annual basis under the No CCS and Ambitious  $H_2$  scenarios is shown, where the periods when policies are in place are shaded. As expected, R&D has limited immediate impact on sales when it is applied (2020-2024) and only seen later by providing a higher starting point (4.6 vs. 1.6 million FCEV as part of the car stock) when the rest of the policies come in place in 2030. The combined effect of fuel, infrastructure and purchase subsidies results in the increase of sales to 9 million FCEV a year by the end of the period (2034) compared to only 1.8 million FCEV in the No CCS scenario. Even though sales drop to 4 million a year as soon as the incentives are removed, these FCEV sales stay 1.5-2 million higher than the No CCS scenario, which translates into an offset of 25-30 more million FCEV in the car stock post-2030 and changing the 2050 share from 16.4% in the No CCS to 26.4% in the Ambitious  $H_2$  (Fig. 12b). In combination with very stringent CO<sub>2</sub> targets, the proposed FCEV policy package leads to a situation where FCEV becomes the most widespread powertrain technology in the European car market in 2050 (see Fig. SI 18 in Appendix 5 for the car stock composition by MS for this Ambitious  $H_2$  scenario).

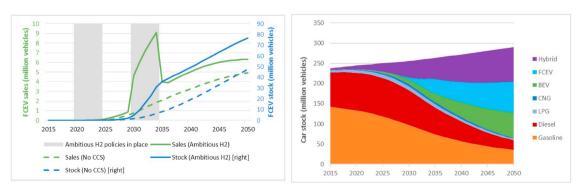


Fig. 12. PTTMAM simulations: (a) EU28 FCEV sales and stock for the No CCS and Ambitious  $H_2$  scenarios; (b) EU28 powertrain mix for the Ambitious  $H_2$  scenario.

**Table 6**Effect of timing and level of policy support on EU28 FCEV cumulative sales (million vehicles sold 2015–2050).

Policy	Policy instrument value	Implementation period/FCEV cumulative sales			
		2020–2024	2025–2029	2030–2034	
No policy	-		67		
(P1) Purchase subs authority	25%	67.4	67	N/A	
(P2) Purchase subs OEM	5 k€	72.9	76.2	91.3	
(P3) Purchase subs auth + OEM	25%/5 k€	74.3	76.2	91.3	
(P4) Infras inv + fuel subs	100%/100%	67.3	70.8	81	
(P5) R&D (FC + tank)	2.5 bln€/2.5 bln€	72.6	69.7	67	
(P6) R&D (FC only)	5 bln€	77.5	71.5	67	
Ambitious H <sub>2</sub>	P1 + P2 + P4 + P6		123.5		

#### 7. Conclusions

With the challenges of lower CO2 emissions and a more integrated energy system with increased sector coupling, there is a need for using more overarching models that capture the various interdependencies of the energy system. Transport models need to consider the interaction with the rest of the energy system through commodity prices, resource constraints and energy supply while energy models need to consider the intricacies of the choices in the transport sector. The literature review in this study showed that there are multiple efforts to bring these two types of models together, where lessons can also be drawn from similar engineering models such as Integrated Assessment Models. This study looked at one potential alternative to bridge these two worlds by softlinking a system dynamics model with an energy system model applied specifically for FCEV in a 2050 future with 80-95% CO2 reduction for the entire energy system. Two approaches for this soft-linking were explored, one feeding back the powertrain shares from the simulation to the optimization model and one where the cost for the various powertrains was the parameter exchanged. It was found that the most useful approach is when the shares are fed back. This enables exploiting the behavioral aspect of the end users that is part of the simulation model, it avoids large swings in shares characteristic of the optimization model and it still captures the interaction with the rest of the energy system.

In turn, two approaches to feed back the shares were explored, one with the shares at EU level (leaving the choice of country shares to the optimization framework) and one with fixed country shares (i.e. less flexibility). The benefit of doing it at EU level were limited. The cumulative costs (2015–2050) were 0.5% lower and on average 0.4 €/kg cheaper hydrogen (compared to an average  $\rm H_2$  price of 5 €/kg) when shares at EU level were used. However, large swings of up 70–80% in powertrain shares for individual countries were observed. In this approach, FCEV started to be deployed earlier (before 2030). In this early period, it was more attractive to use gas reforming combined with  $\rm CO_2$  storage to produce relatively cheap hydrogen and only later on when FCEV and refueling stations have become cheaper use electrolysis as main production technology.

Policies that promote FCEV were also analyzed including purchase (by government and manufacturers), fuel, R&D and infrastructure incentives. Their effect was quantified in terms of change in cumulative sales over the 2015–2050 period. A no-policy scenario had 67 million FCEV sales by 2050 to reach a stock of almost 45 million FCEV. The measure with the largest net impact was a vehicle discount by manufacturers of 5 k€ per vehicle. This had a total cost of 84 bln€ with a net effect of 24.3 additional million FCEV sold. A 5 bln€ invested in R&D resulted in 10.5 additional million FCEV, while 113 bln€ in infrastructure and fuel subsidy only increased the cumulative FCEV sales by 14 million. The timing of each policy had a large impact, where R&D had the highest impact in the 2020–2024 period, while the rest of incentives were the most effective in 2030–2034. The combination of these policies led to 123 million cumulative sales with an annual peak of 9 million resulting in a FCEV stock of 76.8 million by 2050, which

represent 26.4% of the total car stock, at a cost of 252 bln€. This is to be compared with 47.8 million FCEV (by 2050) in a scenario where no incentive scheme is in place.

Soft-linking introduces the need for iterations and increases the complexity to produce multiple scenarios and analyze the results. Nevertheless, the aforementioned benefits outweigh these costs and soft-linking is overall beneficial. Further research on improving the two models as well as on policy analysis and design by building additional policy scenarios is needed. Future expansions of the modeling framework could include features such as: modal shift, demand split by distance traveled, consideration of travel time budget, consideration of a second hand market, spillover effect of other transport sectors over battery and fuel cell costs, different car use pattern for households with multiple cars and higher heterogeneity in terms of consumer attributes, while applying this framework to ambitious CO2 scenarios with new energy carriers such as hydrogen. In addition, more research needs to be undertaken to improve the understanding of behavioral dynamics and their representation in models. This study only covers the use of hydrogen for cars which should be evaluated in the broader context of transport and potential hydrogen (or derivatives) use for heavy-duty, trains, ships and planes where its potential can be high due to its higher energy density (vs. electricity).

#### Appendix A. Supplementary data

Supplementary data to this article can be found online at https://doi.org/10.1016/j.rser.2019.109349.

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