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The Role of Electricity in Decarbonizing European Road Transport – Development and Assessment of an Integrated Multi-Sectoral Model

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Abstract

Despite regulation efforts, CO_2 emissions from European road transport have continued to rise. Increased use of electricity offers a promising decarbonization option, both to fuel electric vehicles and run powerto-x systems producing synthetic fuels. To understand the economic implications of increased coupling of the road transport and electricity sectors, an integrated multi-sectoral partial-equilibrium investment and dispatch model is developed for the European electricity and road transport sectors, linked by an energy transformation module to endogenously account for, e.g., increasing electricity consumption and flexibility provision from electric vehicles and power-to-x systems. The model is applied to analyze the effects of sectorspecific CO_2 reduction targets on the vehicle, electricity and ptx technology mix as well as trade flows of ptx fuels in European countries from 2020 to 2050. The results show that, by 2050, the fuel shares of electricity and ptx fuels in the European road transport sector reach 37% and 27%, respectively, creating an additional electricity demand of 1200 TWh in Europe. To assess the added value of the integrated modeling approach, an additional analysis is performed in which all endogenous ties between sectors are removed. The results show that by decoupling the two sectors, the total system costs may be significantly overestimated and the production costs of ptx fuels may be inaccurately approximated, which may affect the merit order of decarbonization options.

Keywords: Energy system modeling, Electricity sector, Road transport, Power-to-x, Synthetic fuels, Sector coupling, Decarbonization

JEL classification: C61, N70, Q41, Q42, Q48, R42

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1. Introduction

Preventing severe, pervasive and irreversible impacts of climate change requires rapid emission reduction in all sectors (IPCC (2014)). However, European road transport emissions have increased by 22% since 1990, accounting for a share of 21% of total European greenhouse gas emissions in 2016 (EEA (2018)). European regulation such as fleet targets for the average carbon emission levels for new vehicles is one of the more recent attempts to decarbonize road transport; however, factors such as increasing road transport demand and the countinued adoption of fossil-fueled gasoline and diesel motors have counteracted emission reduction efforts. Diversification of the current fuel and vehicle mix using alternatives such as natural gas, hydrogen, biofuels, synthetic fuels and electricity would offer decarbonization opportunities – yet the cost-optimal pathway to a low-carbon fuel mix remains unclear.

Most recently, electricity has gained attention as an energy carrier capable not only of fueling electric vehicles but also power-to-x (ptx) systems to produce synthetic power-to-x fuels (ptx fuels). More specifically, stand-alone electrolysis or electrolysis coupled with, e.g., methanation or Fischer-Tropsch synthesis can produce zero-carbon and carbon-neutral fuels for the road transport sector.¹ Yet decarbonizing the road transport sector via electricity results in the road transport and electricity sectors being coupled such that supply and demand become linked across sectors, which may have significant impacts on the future energy system. On the one hand, increased electricity consumption from road transport and ptx systems would require additional electricity generation, which must be produced subject to its own emission reduction regulations. In this case, both the marginal cost of electricity demand from road transport and ptx systems systems. On the other hand, linking the road transport and electricity sectors may provide system flexibility since, e.g., electric vehicles or electrolysis may serve as energy storage capacities for the electricity sector. Especially in the case of high variable renewable energy (VRE) deployment, power-to-x systems may consume electricity in hours of high VRE supply and very low or even negative electricity prices as well as may offer ptx fuels to generate electricity in times of poor VRE supply and critical demand.

With growing pressure for decarbonization and an increased interest in electrification, it becomes vital to understand the economic implications of coupling the road transport and electricity sectors. One common method to assess long-term market behavior is via numerical optimization models, which assume future developments in, e.g., emissions, electricity demand and technologies. However, many current modeling

 $^{^{1}}$ Zero-carbon fuels refers to fuels with a chemical composition without C-atoms and thus with no carbon emissions associated when burnt. Carbon-neutral fuels, however, generate carbon emissions during combustion, but consist of recycled carbon and thus form part of the carbon cycle (see Section 2.1.5 for a more detailed discussion).

approaches tend to either focus on a single sector or on the energy system as a whole. As such, they either fall short of accounting for cross-sectoral interdependencies or lack granularity in their representation of technologies regarding, e.g., road transport and energy transformation such as power to x. Therefore, the paper at hand seeks to answer the following research questions: i) how can the road transport sector and energy transformation technologies be integrated into an electricity market model?, ii) what are the key interactions between the sectors and technologies, and how may these contribute to decarbonization?, and iii) what is the added value of modeling the electricity and road transport sectors as well as energy transformation processes in an integrated multi-sectoral framework?

Within the scope of this paper, an integrated multi-sectoral partial-equilibrium investment and dispatch model combining the European electricity and road transport sectors is developed. A linear dynamic electricity market optimization model is extended to include both the European road transport sector in a road transport module as well as cross-sectional conversion technologies such as power-to-x systems, with the x indicating a synthetic gas or fuel, in an energy transformation module. The focus lies not only on creating a detailed technological representation within each module but also on properly accounting for any interconnections between the electricity and road transport sectors as well as energy transformation processes. These include all electricity consumption from electric mobility or from energy transformation as well as ptx fuel flows to the road transport and electricity sectors, both within countries and across borders. Furthermore, the model observes any cross-sectoral emissions, such as upstream emissions in the electricity sector emitted during electricity generation for the road transport sector. Many cross-sectoral technologies such as power-to-x systems may only become competitive if they can be rewarded for their carbon-neutral nature, which is only apparent when considering the complete emissions cycle of the fuel production pathway.

The extended integrated multi-sectoral model is then able to simulate cost-minimal decarbonization pathways for the electricity and road transport sectors in European countries up to 2050. In order to demonstrate the capabilities of the model developed, an exemplary scenario is presented to analyze the effects of sector-specific CO_2 reduction targets on the long-term vehicle, electricity and ptx technology mix in Europe. The model yields the cost-optimal solution, minimizing the total costs of the electricity sector as well as the total costs for the vehicles, fuel use and infrastructure needed to reach the CO_2 reduction goals. The results of the single scenario analysis show that, by 2050, the fuel share of electricity and ptx fuels in the European road transport sector reaches 37% and 27%, respectively, creating an additional electricity demand of 1200 TWh in Europe. The scenario results provide a basis for understanding the integrated multi-sectoral model, revealing endogenous marginal costs of electricity generation and sectorspecific marginal CO_2 abatement costs as well as cross-border trade flows that reflect the cost-optimal decarbonization pathway under integrated sectors.

In order to understand the added value of building complex integrated models, the second part of the analysis applies the model with decoupled sectors, removing all endogenous ties between the modules and allowing each to be optimized independently of one another. Additional electricity demanded by road transport and energy transformation is therefore ignored by the electricity sector. Electricity prices for the road transport module are defined exogenously. The energy transformation module, which is by definition coupled to the electricity sector, is shut off; however power-to-x fuels can be bought by either the electricity or road transport sector at a fixed price equal to the expected production costs. The results show that by decoupling the two sectors, the total system costs may be significantly overestimated and the production costs of ptx fuels inaccurately approximated, which may affect the merit order of decarbonization options. By comparing the model results, conclusions may be made as to the added value of integrated multi-sectoral modeling and the key discrepancies that may occur when performing single-sector analyses.

This paper is related to two streams of literature. The first relevant stream encompasses research that develops multi-sectoral models covering electricity, road transport and energy transformation. In particular, a large body of literature seeks to extend the MARKAL family of models² to include additional sectors and technologies, with a smaller niche addressing electrification of road transport and power-to-x fuels. Dodds and McDowall (2014) and Dodds and Ekins (2014) extend the MARKAL model to simulate the road transport sector in the UK, with a particular focus on hydrogen consumption. Similarly, Börjesson and Ahlgren (2012) develop and integrate a transport module into MARKAL for the Nordic regions in order to asses taxation strategies. Two other MARKAL models, namely TIMES and TIAM, are also often seen in literature on coupling the road transport and electricity sectors. Both Sgobbi et al. (2016) and Thiel et al. (2016) extend the TIMES model developed in Simoes et al. (2013) to simulate road transport in Europe with approximately 50 vehicle technologies, assessing decarbonization with hydrogen and electricity, respectively. Studies by van der Zwaan et al. (2013) and Rösler et al. (2014) build on the TIAM model described in Rösler et al. (2011) to perform an integrated assessment of decarbonizing the global and European road transport sector, comparing endogenous CO₂ prices across sectors. Apart from MARKAL-based analyses, other simulations of the electricity and road transport sectors include papers by Hedenus et al. (2010) and Krishnan et al. (2014), who build on the models GET 7.0 and NETPLAN, respectively, to determine the

 $^{^{2}}$ The MARKAL (Market Allocation) family of models, including GMM, TIMES and TIAM, were some of the first energy system models (early contributions include Fishbone and Abilock (1981)). MARKAL and its descendants are widely-applied partial equilibrium, bottom-up, dynamic optimization models that are used to identify the energy system meeting energy service demands with the lowest discounted capital, operating and resource costs (Loulou et al. (2004), Dodds and Ekins (2014)).

future vehicle mix and fuel supply under carbon constraints.

Although many of the aforementioned studies use modeling techniques to address similar issues to the study at hand, none of the methodologies were found to implement the same level of temporal, spatial and technological granularity. Often only hydrogen production via electrolysis and the direct use of electricity appear to be coupled to the electricity sector, ignoring the production of other ptx fuels. The possibility to use ptx fuels to decarbonize the electricity sector next to the road transport sector is also not taken into account. Furthermore, the dispatch of ptx technologies is often exogenous, i.e., the utilization rate of, e.g., an electrolysis system is exogenously defined while its investments are endogenous. In the model developed in this paper, ptx systems are exposed to developments in the electricity system at a higher temporal resolution than in the models mentioned. Trade flows of ptx fuels were also found to be possible in only a limited number of cases and are never examined in detail. As such, the study at hand seeks to contribute to the literature on integrated electricity and road transport sector models by accounting for a wide range of ptx applications, optimizing European electricity and ptx fuel production as well as simulating cost-minimizing trade flows according to endogenous market conditions.

The second relevant literature stream focuses on single-sector analyses of the road transport sector and the resulting optimal decarbonization pathways. Many studies assess the penetration of alternative vehicle technologies under certain scenarios (e.g., Pasaoglu et al. (2016), Harrison et al. (2016)). Ou et al. (2013) as well as Gambhir et al. (2015) simulate the Chinese road transport sector up to 2050 to determine total costs under varying penetration levels of electric or hydrogen fuel-cell vehicles. Applying similar methods to those used in the road transport module developed in this paper, Romejko and Nakano (2017) perform a cost minimization for the Polish road transport sector in order to determine endogenous vehicle investments and carbon emissions up to 2030. However, as the models used are decoupled from the energy system, all three papers must assume exogenous prices for all fuels, including electricity. One aim of the study at hand is to gain understanding as to how exogenous assumptions on cross-sectoral parameters may cause the model to deviate from the cost-optimal solution. The assessment of the added value of coupled models, a step that none of the aforementioned studies perform, is another key contribution of this paper.

The remainder of the paper is organized as follows: In Section 2, the methodology behind the coupling of the electricity market, energy transformation and road transport modules as well as behind the individual modules are explained in detail. The scenario framework and results of the integrated model are presented in Section 3, and the comparison to a decoupled model is made in Section 4. Section 5 concludes.³

 $^{^3 \}mathrm{See}$ Appendix A for a list of abbreviations and nomenclature used throughout this paper.

2. Methodology

One of the main objectives of the research at hand is to develop a consistent, integrated energy system model. The foundation of the work presented is the electricity market model DIMENSION, which has been used in numerous analyses;⁴ yet with increasing electrification in synthetic fuel production and road transport, complex interactions arise that cannot be investigated with a single-sector model. In order to account for these multi-sectoral effects, not only do the energy transformation and road transport modules themselves need to be modeled in detail, it is also critical that any interdependencies with the electricity market are also properly simulated.

The remainder of this section is structured as follows: Section 2.1 begins by providing an overview of the model developed in this study as well as identifies the key links connecting the individual modules. The main equations, assumptions and parameters for the energy transformation and road transport modules are then given in Sections 2.2 and 2.3, respectively. For completeness, a short overview of the electricity market module is also included in Appendix B.

2.1. Developing an integrated multi-sectoral model

2.1.1. Overview of the model

Figure 1 presents an overview of the model developed and shows how the individual modules (electricity market, energy transformation and road transport) are connected on the supply side. A key factor of this analysis is that the entire fuel supply chain, from the primary energy source to final fuel consumed, is taken into account. The different fuel types and their production paths can be seen in Figure 1.

The electricity market module, as shown in the yellow area of Figure 1, is responsible for providing the necessary investments to supply electricity to meet both a country-specific exogenous electricity demand⁵ (indicated by the black box) as well as any electricity-consuming technologies in both the energy transformation module (the blue area of Figure 1) or the road transport module (the red area of Figure 1). The yellow lines exiting the yellow area of the electricity market module indicate these electricity flows. The green and gray boxes are the renewable/bio and fossil fuels, respectively, that are available to the power plant fleet.⁶

⁴See, e.g., Jägemann et al. (2013), Knaut et al. (2016) and Peter and Wagner (2018).

⁵The electricity market module is also subject to an endogenous electricity demand from, e.g., storage or demand side response (see Appendix B). For simplification, this is excluded from Figure 1.

 $^{^{6}}$ Investments in nuclear power are only allowed in countries with no existing nuclear phase-out policies. Investments in carbon capture and storage (CCS) technologies are not allowed due to a general lack of social acceptance in European countries.



Figure 1: Overview of the model developed for this study. The yellow area indicates the electricity market module, the blue area the energy transformation module and the red area the road transport module.

The energy transformation module (the blue area) installs power-to-x as well as liquefaction capacities. The blue boxes in Figure 1 show the different ptx processes that are accounted for in the energy transformation module, including electrolysis, CO₂ air capture, methanation, Fischer-Tropsch synthesis as well as hydrogen and methane/gas liquefaction.⁷ Endothermic processes such as electrolysis, which splits water into oxygen and hydrogen, and liquefaction require an electricity input from the electricity market module, as indicated by the yellow lines. The blue lines indicate the flow of ptx fuels, which include zero-carbon ptx hydrogen gas (PtX H2) and ptx liquefied hydrogen (PtX LH2) as well as carbon-neutral ptx methane gas (PtX CH4), ptx liquid methane (PtX LCH4) as well as ptx synthetic gasoline (PtX Gasoline) and ptx synthetic diesel (PtX Diesel).⁸ The dark green boxes and lines depict the production of a gas mixture (Gas Mix), created by feeding in zero-carbon hydrogen from the electrolysis system into the existing natural gas grid.⁹ The resulting gas mixture is equivalent to a low-carbon substitute for fossil natural gas and can also

⁷Unlike the other processes presented, CO₂ air capture is not modeled as an investment object but rather assumed to be available at a feedstock price equal to the average costs of CO₂ air capture (see Section 2.2.1).

 $^{^{8}}$ The upstream emissions from the electricity generation used as input for the ptx production processes are accounted for within the electricity market emissions. Therefore, the zero-carbon and carbon-neutral properties hold with respect to the sector in which the fuel is used, irrespective of how the electricity was generated in the first place. See Section 2.1.5 for a detailed discussion.

 $^{^{9}}$ The existing natural gas grid is not modeled as an investment object but rather as an energy constraint (see Section 2.2.1).

be liquefied via methane/gas liquefaction to provide a low-carbon alternative to fossil liquefied natural gas (Liq. Gas Mix). The energy transformation module is not subject to an exogenous demand but rather optimizes its supply according to the other modules, meaning that ptx fuels can either be supplied back to the electricity market module (i.e., as ptx methane or gas mix for electricity generation) or to the road transport module to be used in a wide range of vehicle technologies.

The road transport module invests in vehicle technologies as well as infrastructure to cover an exogenous demand for road transport (indicated by the black box), varying across countries and years. In the model, the equilibrium condition is defined in annual vehicle kilometers, which in turn defines an energy demand based on the vehicle's motor type and specific fuel consumption. As indicated by the red lines, a single vehicle technology may consume multiple fuel types, as explained in Section 2.1.4. In addition to ptx fuels (blue and dark green boxes), the road transport module may also purchase fossil fuels (gray boxes) such as gasoline, diesel, natural gas (CNG), liquefied natural gas (LNG), hydrogen gas (H2) and liquefied hydrogen (LH2) from natural gas reformation as well as biofuels (light green boxes) such as biodiesel, biogasoline, biogas and bio LNG. Fossil fuels and biofuels can be bought from the global commodity market at a price reflecting both the raw fuel and the fuel production costs.¹⁰ Electricity may also be consumed in the road transport module, which is endogenously supplied by the electricity market module.

The integrated multi-sectoral model optimizes the energy transformation and road transport modules simultaneously with the electricity market module to determine the cost-efficient investment and dispatch strategy for meeting electricity and road transport demand of each country. To this end, accumulated discounted total system costs are minimized subject to regulatory conditions as well as technical constraints such as carbon emission reduction targets¹¹ or energy balance restrictions. The model allows for an integrated analysis yielding a cost-minimal, welfare-optimal solution across multiple coupled sectors. The spatial scope of the model covers 28 countries, including 26 countries of the European Union as well as Norway and Switzerland.¹² The analyzed time period spans 2015 to 2050 in 5-year steps. For computational tractability, the model applies a reduced temporal resolution based on 16 typical days.¹³

 $^{^{10}}$ Costs for oil refining, natural gas reformation, etc. are added as a price markup to the commodity price. Note that such a marginal cost approach does not take into account any sunk costs such as the investment costs for oil refineries. Biofuels are assumed to be traded on a European market, with prices based on the fossil-based equivalent plus a 20% markup.

 $^{^{11}}$ In its current form, the model only considers CO₂ emissions and does not account for other externalities such as air pollution and resulting health damage.

¹²See Table A.2 in Appendix A for a complete list of the countries considered.

 $^{^{13}}$ In order to represent a full year, the typical days are scaled up by multiplying each typical day with its frequency of occurrence. Each typical day consists of four time slices representing six consecutive hours. The authors have chosen this temporal resolution due to restrictions in computational power given the complexity of the multi-sectoral model framework. As shown in Nahmmacher et al. (2016), a temporal resolution exceeding 48 time slices is assumed to be sufficient to ensure reliable results when using investment models for electricity.

2.1.2. Understanding the structure of the electricity market module

The model developed within the scope of this study is an extended version of the dynamic electricity market model DIMENSION, similar to the integrated problem for investment and operation as presented in, e.g., Turvey and Anderson (1977). It may be interpreted as a social planner problem in which the social planner minimizes total system costs under perfect foresight for investments in generation capacity and the operation of generation and transmission between markets.¹⁴

As is often seen in the literature on electricity market modeling, fundamental assumptions are necessary to reduce the complexity of the optimization problem. The model at hand assumes inelastic demand due to, e.g., the lack of real-time pricing as well as market clearing under perfect competition. As such, the problem can be treated as a linear optimization, as shown in Equation (1). The objective function (1a) minimizes total costs TC, i.e., the sum of the fixed costs of generation capacity $\bar{\mathbf{x}}_{i,m}$ and variable costs of generation $\mathbf{g}_{i,m,t}$ of technology i in market m.¹⁵ Investing in additional generation capacities comes with costs of $\delta_{i,m}$ and generation incurs variable costs of $\gamma_{i,m,t}$.

min
$$TC = \sum_{i,m} \delta_{i,m} \bar{\mathbf{x}}_{i,m} + \sum_{i,m,t} \gamma_{i,m,t} \mathbf{g}_{i,m,t}$$
 (1a)

s.t.
$$l_{m,t} = \sum_{i} \mathbf{g}_{i,m,t} + \sum_{n} \mathbf{k}_{n,m,t} \qquad \forall m, t, m \neq n$$
 (1b)

$$\mathbf{g}_{i,m,t} \le x_{i,m,t} \mathbf{\bar{x}}_{i,m} \qquad \qquad \forall i,m,t \qquad (1c)$$

$$|\mathbf{k}_{m,n,t}| \le \bar{k}_{m,n} \qquad \qquad \forall m, n, t, m \ne n \tag{1d}$$

$$\mathbf{k}_{m,n,t} = -\mathbf{k}_{n,m,t} \qquad \qquad \forall m, n, t, m \neq n \tag{1e}$$

$$l_{m,peak} \le \sum_{i} v_{i,m} \bar{\mathbf{x}}_{i,m} \qquad \forall m \tag{1f}$$

$$GHG_{cap} \ge \sum_{i,m,t} \kappa_i \mathbf{g}_{i,m,t} / \eta_{i,m}$$
 (1g)

for technologies $i \in \mathbf{I}$, markets $m, n \in \mathbf{M}$ and time $t \in \mathbf{T}$.

The cost-minimizing objective function is subject to various constraints: The equilibrium condition (1b) ensures that supply, i.e., the sum of generation $\mathbf{g}_{i,m,t}$ and electricity exchanges between markets m and n, $\mathbf{k}_{n,m,t}$ and $\mathbf{k}_{m,n,t}$, equals demand $l_{m,t}$. The two capacity constraints (1c) and (1d) require that generation

 $^{^{14}}$ The electricity market model DIMENSION will be referred to as the *electricity market module* henceforth. The reader is referred to Richter (2011), Fürsch et al. (2013) and Jägemann et al. (2013) for more detailed descriptions of the model DIMENSION, which was developed and has been maintained at the Institute of Energy Economics at the University of Cologne (EWI).

 $^{^{15}}$ See Table A.1 in Appendix A for a complete list of model sets, parameters and variables. Unless otherwise noted, bold capital letters indicate sets, lowercase letters parameters and bold lowercase letters for optimization variables.

and transmission are restricted by installed generation and transmission capacities. Equation (1e) states that electricity trades from market m to market n are equal to negative trades from market n to market m. The peak capacity constraint (1f) requires the sum of generation capacities $\bar{\mathbf{x}}$ weighted by their capacity values¹⁶ $v_{i,m}$ is to be greater than or equal to the market-specific annual peak load $l_{m,peak}$. The peak capacity constraint is typically introduced in long-term investment models that are based on a reduced temporal resolution, e.g., a typical-days approach, to ensure security of supply even when only modeling select hours. Finally, the decarbonization constraint (1g) requires the sum of greenhouse gas emissions of all technologies in all markets to be lower than a certain greenhouse gas cap. The emissions are calculated by dividing electricity generation $\mathbf{g}_{i,m,t}$ by the technology-specific efficiency $\eta_{i,m}$ to determine the technology's fuel consumption, which is then multiplied with its fuel-specific emission factor κ_i .

2.1.3. Identifying key links between modules

Within the scope of this research, two additional modules were developed and embedded into the optimization problem shown in Equation (1): a road transport module simulating the European road transport sector and an energy transformation module simulating conversion technologies, e.g., power-to-x systems providing fuels to the electricity and road transport sectors.

The complexity of a multi-sectoral model lies within the proper representation of interlinkages between the modules.¹⁷ Within the integrated multi-sectoral model, the electricity market module is still represented by Equations (1b) - (1f), which now, however, only apply to the set of electricity market technologies $i \in \mathbf{I}_{el}$, i.e., a sub-quantity of the entire quantity of technologies $\mathbf{I} = \mathbf{I_{el}} + \mathbf{I_{rt}} + \mathbf{I_{et}}$ comprising all technologies from the electricity market module, the road transport module and the energy transformation module.

The cost-minimizing objective function (1a) is still valid; however it now encompasses technologies from all modules, i.e., $i \in \mathbf{I}$, and thereby represents the core of the integrated modeling approach. The fixed costs $\delta_{i,m}$ include the annuity as well as the yearly fixed operation and maintenance costs of power plants, vehicles and infrastructure as well as ptx and liquefaction systems. The variable costs $\gamma_{i,m,t}$ include fuel costs as well as costs for, e.g., CO_2 air capture and fuel distribution (see Sections 2.2.1 and 2.3.1).

One key link between the modules is achieved via modifying the equilibrium condition (1b) in order to account for the endogenous electricity demand from all modules. In addition to the endogenous electricity demand in the electricity market module, e.g., by storage technologies, both the energy transformation

 $^{^{16}}$ In the existing literature, capacity value and capacity credit are often used as synonyms. Throughout this paper, the term capacity value is used. $^{17}{\rm See}$ Figure C.1 in Appendix C for a schematic representation of the key links between the modules.

module and the road transport module may demand electricity in order to generate ptx fuels (see Section 2.2.3) or fuel electric vehicles (see Section 2.3.3), which in turn must be supplied by the electricity market module. The modified equilibrium condition then reads

$$l_{m,t} + \sum_{s} \mathbf{ec}_{f,f1,m,s,t} \bigg|_{f,f1=elec} = \sum_{i} \mathbf{g}_{i,m,t} + \sum_{n} \mathbf{k}_{m,n,t}$$
(2)

where the electricity demand has both an exogenous component, $l_{m,t}$, and an endogenous component, represented by the electric energy consumption $\mathbf{ec}_{f,f1,m,s,t}$ for f1 = f = electricity, summed over sectors s.

Another key link between the modules is the endogenous country-specific electricity price. It is implicitly visible to all modules as they are all subject to one common cost-minimizing objective function (1a). The endogenous country-specific electricity price is derived from the dual variable of Equation (2) and represents the change in total system costs for supplying one additional unit of electricity. The remaining two key links between the modules consist of the endogenous ptx fuels demand and the resulting endogenous ptx fuel price in the energy transformation module: The endogenous ptx fuel demand drives investments in ptx and liquefaction technologies, which in turn determines the implicit ptx fuel prices, discussed in Section 2.2.3.

2.1.4. Introducing substitute fuels

Both the electricity market module and road transport module have a wide range of fuels to choose from when making the investment decision in an electricity generation or vehicle technology. However, some of the fuel choices are substitutes, varying only in, e.g., production costs and upstream carbon emissions. For example, a fuel-cell vehicle running on hydrogen can run both on ptx and fossil-based hydrogen; yet the model must be able to distinguish between the two fuel types as hydrogen from electrolysis differs strongly in terms of production cost and upstream carbon emissions compared to that from natural gas reformation. Moreover, both carbon-based ptx fuels and biofuels are assumed to be carbon neutral, which can only be accounted for if the fuel's production cycle is properly recognized by the model (see Section 2.1.5).

As a result, the concept of substitute fuels is introduced in order to differentiate fuels by how they are produced while still allowing for fuels to be grouped by their type (Table 1).¹⁸ It should be noted that for fuels without multiple substitute fuels (e.g., electricity, coal, lignite), f equals f1. For simplification they are omitted from Table 1.

 $^{^{18}}$ It should be noted that the concept of substitute fuels ignores any differences in the chemical composition of the respective fuels. Substitute fuels are thus treated, economically speaking, as perfect substitutes. This assumption is justified in an economic model as long as the fuel-consuming technologies can interchangeably switch between fuels without affecting their performance.

Fuel type f	Substitute fuels f_1		
Diesel	Diesel	PtX Diesel	Biodiesel
Gasoline	Gasoline	PtX Gasoline	Biogasoline
Gas	CNG	PtX CH4/Gas Mix	Biogas
Liquefied Gas	LNG	PtX LCH4/Liq. Gas Mix	Bio LNG
Hydrogen	H2	PtX H2	
Liquefied Hydrogen	LH2	PtX LH2	

Table 1: Fuel types and the corresponding substitute fuels

By applying the concept of substitute fuels, not only can each sector's endogenous energy consumption $\mathbf{ec}_{f,f1,m,s,t}$ be determined for a certain fuel type f, but the mix of substitute fuels f1 can be simultanously derived, taking into account constraints such as decarbonization targets. As such, in terms of the electricity market model given in Equation (1), the energy consumption of power plants in the electricity sector is then defined by

$$\sum_{f1} \mathbf{ec}_{f,f1,m,s,t} \bigg|_{s=el} = \sum_{i} \mathbf{g}_{i,m,t} / \eta_{i,m} \qquad \forall m,t,f.$$
(3)

For example, the ptx methane consumption of a power plant in the electricity sector s = el of market m is depicted by $\mathbf{ec}_{f,f1,m,s,t}$ with f = gas and f1 = ptx methane. The electricity consumption of, e.g., a pump storage is denoted by f1 = f = electricity.

2.1.5. Accounting for upstream emissions and the carbon cycle

Carbon emissions from combustion processes are based on the carbon content of the respective fuel, i.e., a fuel-specific carbon emission factor κ_{f1} . For non-carbon fuels such as electricity or hydrogen, this value is equal to zero. Fuel-specific upstream carbon emissions, on the other hand, include emissions from fuel extraction and transformation and are accounted for by a fuel-specific upstream carbon emission factor $\kappa_{f1,upstream}$.¹⁹ For fossil fuels and biofuels, this includes carbon emissions generated during fuel production and conditioning at the source, fuel transformation at the source, transformation near market and conditioning and distribution (Edwards et al. (2014)).²⁰ It should be noted that the upstream emissions of electricity as an input fuel for, e.g., electric vehicles or ptx processes are accounted for in the electricity market module.

¹⁹Note that the carbon emission factor from combustion processes κ_{f1} is equal for fuel f and its substitute fuels f1, assuming the fuels are perfect substitutes. The upstream carbon emissions factor $\kappa_{f1,upstream}$ however varies for different substitute fuels f1.

 $^{^{20}}$ Upstream emissions differs from a Life Cycle Analysis (LCA), as it does not consider energy and emissions involved in building facilities and the vehicles, or end of life aspects.

Thus, the upstream emissions of ptx fuels produced in the energy transformation module consist only of emissions resulting from the distribution of the final fuel from the central ptx system to the consumer. The fuel-specific carbon emission factors and upstream carbon emission factors are shown for each substitute fuel in Table D.4 of Appendix D.

The carbon emissions $\mathbf{em}_{m,s}$ from sector s in market m are then defined by

$$\mathbf{em}_{m,s} = \sum_{f,f1,t} \mathbf{ec}_{f,f1,m,s,t} (\kappa_{f1} + \kappa_{f1,upstream}) \qquad \forall m, s.$$
(4)

In order to account for the carbon cycle of carbon-neutral fuels such as biofuels or ptx fuels (discussed in detail in Section 2.2.1), a carbon capture variable $\mathbf{cpt}_{m,s}$ is introduced and defined as

$$\mathbf{cpt}_{m,s} = \sum_{f,f1,t} \mathbf{ec}_{f,f1,m,s,t} \kappa_{f1}|_{f1=bio/ptx} \qquad \forall m,s.$$
(5)

Thereby, it is assumed that the entire carbon content of the biofuels or ptx fuels, represented by κ_{f1} , is captured from air either by natural carbon bonding via biomass photosynthesis or by a direct air capture process (DAC) (see Section 2.2.1). It thus forms a carbon cycle and the respective fuel can be regarded as carbon neutral.

A generalized formulation of the decarbonization constraint (1g) in Equation (1) reads then as

$$GHG_{cap,s} \ge \sum_{m} (\mathbf{em}_{m,s} - \mathbf{cpt}_{m,s}) \qquad \forall s$$
 (6)

It should be noted that for carbon-neutral fuels, i.e., biofuels and ptx fuels, the emissions κ_{f1} cancel out in Equation (6); however, any upstream emissions based on $\kappa_{f1,upstream}$ do not. Furthermore, the sum on the right hand side of Equation (6) has to be adjusted depending on the definition of the decarbonization target, be it a multi-national sectoral target, a national sectoral target, or a national multi-sectoral target.

2.2. Simulating energy transformation

The energy transformation module is a tool that was developed to simulate the investment in as well as energy consumption and production volumes of energy conversion technologies in order to serve, among others, the electricity and road transport sectors. Within the scope of this analysis, the module endogenously reacts to developments in the electricity market (i.e., increased VRE production) as well as the demand for ptx fuels in the electricity and road transport modules, which may be necessary to achieve, e.g., decarbonization targets. This subsection seeks to introduce the conversion technologies considered (Section 2.2.1) as well as provide key details on how the ptx fuel supply is modeled (Section 2.2.2). Further explanation on how the conversion technologies are linked to the electricity market module is provided in Section 2.2.3.

2.2.1. Power-to-x, liquefaction and carbon neutrality via CO_2 air capture

The ptx conversion technologies, analogous to the electricity generation technologies, are investment objects with defined techno-economical parameters that vary across vintage classes. These technologies include alkaline and PEM electrolysis, catalytic methanation and Fischer-Tropsch synthesis. Key techno-economic assumptions for each ptx investment object considered in the energy transformation module including investment costs, fixed operation and maintenance costs (FOM), efficiency and technical lifetime can be found in Table D.5 in Appendix D. Plants to liquefy gaseous hydrogen or natural gas are also taken into account in the energy transformation module. Analogous to ptx systems, liquefaction plants are modeled as investment objects. The techno-economic assumptions for the liquefaction plants may be found in Table D.6 in Appendix D.



Figure 2: Inputs and outputs of ptx processes

Figure 2 gives an overview of the relevant input and outputs for each ptx technology modeled in this analysis. The hydrogen gas produced in electrolysis can either be sold directly or be stored to successively produce methane via catalytic methanation or hydrocarbons via Fischer-Tropsch synthesis. Alternatively, ptx hydrogen may be mixed with natural gas in the existing gas grid infrastructure up to a certain threshold which depends on the design and certification of end appliances. An upper limit of 10 vol-% of the natural gas grid is assumed for hydrogen feed-in.²¹ It should be noted that, as shown in Figure 2, an electrolysis system produces oxygen as by-product. As such, in addition to selling ptx fuels, the energy transformation module also sells oxygen to an exogenously-defined market at an exogenous price, increasing the profitability of ptx systems.²² Detailed descriptions of the energy transformation processes can be found in Appendix D.2.

 $^{^{21}}$ In the future, it is expected that gas turbines, motors and consumer appliances will be able to function under higher shares of hydrogen gas. However, the authors have chosen 10 vol-% as an average in order to account for a wide range of older and newer technologies. In order to set the limit in the model, the national gas demand is used as a proxy for gas grid size in each respective country.

²²An oxygen price of 0.07 EUR/cubic meter is assumed based on Brynolf et al. (2018). The country-specific upper limit

As previously stated, the ptx fuels produced in the energy transformation module are assumed to be either zero-carbon or carbon neutral. Upstream emissions aside, hydrogen fuel produced from electrolysis is by definition carbon-free as electricity splits water into oxygen and hydrogen. Technologies such as methanation and Fischer-Tropsch synthesis, however, produce carbon-based fuels that, via combustion, will emit carbon dioxide into the atmosphere. Yet these ptx fuel production processes require carbon dioxide together with hydrogen as an input in order to create carbon-based ptx methane or ptx gasoline and ptx diesel (see Figure 2). The classification carbon neutral depends on the origin of the carbon fed into the ptx processes. More specifically, if the carbon stems from a fossil-based origin, the eventual release of carbon dioxide during the ptx fuel combustion process cannot be regarded as carbon neutral.²³ If, however, the carbon is based on air capture either from biomass photosynthesis or a technical direct air capture process, the CO_2 is recycled, resulting in a carbon-neutral process being part of a carbon cycle. In this work, it is assumed that the carbon required for ptx fuel production stems from CO_2 extracted from the atmosphere via direct air capture.²⁴

2.2.2. Key aspects of modeling the supply of ptx fuels

The equilibrium condition for ptx fuels ensures that the ptx fuel production, $\mathbf{fp}_{f1,i,m,t}$, within each country m in addition to any ptx fuel trade $\mathbf{ft}_{f1,n,m,t}$, i.e., ptx fuels being imported into country m from other EU countries n or from outside of Europe, $\mathbf{ft}_{f1,nonEU,m,t}$, is equal to the amount of ptx energy consumption in country m, $\mathbf{ec}_{f,f1,m,s,t}$, plus ptx fuel exports from country m to country n, $\mathbf{ft}_{f1,m,n,t}$:

$$\sum_{i} \mathbf{f} \mathbf{p}_{f1,i,m,t} + \sum_{n} \mathbf{f} \mathbf{t}_{f1,n,m,t} + \mathbf{f} \mathbf{t}_{f1,nonEU,m,t}$$
$$= \sum_{s} \mathbf{e} \mathbf{c}_{f,f1,m,s,t} + \sum_{n} \mathbf{f} \mathbf{t}_{f1,m,n,t} \qquad \forall m, t, f, f1.$$
(7)

This equilibrium condition holds for all liquid fuels f1 produced by ptx technologies i such as ptx gasoline, ptx diesel, ptx liquefied hydrogen, ptx liquid methane and liquefied gas mix.

The gaseous ptx fuels, namely ptx hydrogen, ptx methane and gas mix, are subject to a slightly modified equilibrium condition in order to account for any ptx hydrogen that is injected into the natural gas grid.

for oxygen sales is estimated based on industry data for Germany (VCI (2014)) and for the other European countries scaled according to GDP (Eurostat (2017)), whereby only 25% of a country's oxygen demand is assumed to be able to be provided by electrolysis.

 $^{^{23}}$ Note that carbon from fossil-based carbon capture and utilization (CCU) is, while relieving the first combustion process from its carbon emissions, still fossil-based carbon. Thus, it does not qualify for production of carbon-neutral ptx fuels, as this would entail double counting.

 $^{^{24}}$ The CO₂ feedstock prices from air capture are assumed to reduce from 300 EUR/tCO_2 in 2020 to 84 EUR/tCO_2 in 2050 (Sanz-Pérez et al. (2016)), as shown in Figure E.2 in Appendix E.

Similar to Equation (7), the equilibrium conditions for gaseous ptx fuels are

$$\sum_{i} \mathbf{f} \mathbf{p}_{PtXH2,i,m,t} + \sum_{n} \mathbf{f} \mathbf{t}_{PtXH2,n,m,t} + \mathbf{f} \mathbf{t}_{PtXH2,nonEU,m,t}$$
$$= \sum_{s} \mathbf{e} \mathbf{c}_{H2,PtXH2,m,s,t} + \sum_{n} \mathbf{f} \mathbf{t}_{PtXH2,m,n,t}$$
$$+ \mathbf{f} \mathbf{f}_{PtXH2,m,t} \qquad \forall m,t \qquad (8)$$

$$\sum_{i} \mathbf{f} \mathbf{p}_{PtXCH4,i,m,t} + \sum_{n} \mathbf{f} \mathbf{t}_{PtXCH4/GasMix,n,m,t} + \mathbf{f} \mathbf{t}_{PtXCH4,nonEU,m,t} + \mathbf{f} \mathbf{f}_{PtXH2,m,t}$$

$$= \sum_{s} \mathbf{e} \mathbf{c}_{Gas,PtXCH4/GasMix,m,s,t}$$

$$+ \sum_{n} \mathbf{f} \mathbf{t}_{PtXCH4/GasMix,m,n,t} \quad \forall m,t \qquad (9)$$

with the extra variable ptx fuel feed-in $\mathbf{ffi}_{PtXH2,m,t}$ indicating the amount of ptx hydrogen injected into the natural gas grid. In Equation (8), the ptx hydrogen into grid contributes to the hydrogen demand, whereas in Equation (9) it becomes part of the gas supply. Apart from being fed into the natural gas grid ($\mathbf{ffi}_{PtXH2,m,t}$), ptx hydrogen can be directly used in sectors such as road transport or sent to a liquefaction plant in order to produce ptx liquefied hydrogen ($\mathbf{ec}_{H2,PtXH2,m,s,t}$). Ptx methane, analogous to ptx hydrogen, can be either fed into the natural gas grid or liquefied, represented by each sector 's energy consumption ($\mathbf{ec}_{Gas,PtXCH4/GasMix,m,s,t}$).²⁵

As shown in Equation (7), (8) and (9), ptx fuels can either be traded between European countries or bought from outside of Europe, e.g., from North Africa. Inner-European import and export volumes via trucks are determined endogenously, being subject to tanker transport costs relative to delivery distance.²⁶ As the model does not cover investments outside Europe, an exogenous ptx fuel import price is calculated based on the expected production and distribution costs of ptx fuels at a typical location in North Africa.²⁷ For the recycled carbon supply for ptx diesel, ptx gasoline and ptx methane production outside of Europe, CO_2 air capture is assumed and included in the production costs. Ptx fuels from European production are not permitted to be exported outside Europe.

 $^{^{25}}$ Note that liquefaction plants use gaseous ptx hydrogen and ptx methane as input, representing an energy consumption of the energy transformation module in Equations (8) and (9).

²⁶The transport costs are derived based on km-specific transport costs and the distance between capital cities as a proxy, see Table D.7 in Appendix D.

 $^{^{27}}$ The production costs include the investment and FOM costs of the ptx systems as well as the variable costs, i.e., the electricity price, calculated as the LCOE of a hybrid onshore wind and photovoltaics plant in North Africa.

2.2.3. Linking the energy transformation module to the electricity market and road transport modules

One key link between the energy transformation and electricity market module is the demand of electricity by power-to-x and liquefaction systems to produce gaseous and liquid ptx fuels, determined endogenously. The electric energy consumption $\mathbf{ec}_{f,f1,m,s,t}$ of the energy transformation module is defined as

$$\sum_{f1} \mathbf{ec}_{f,f1,m,s,t} \bigg|_{f,f1=elec} = \sum_{i} \mathbf{fp}_{f1,i,m,t} / \eta_{i,m} \qquad \forall m,t \qquad (10)$$

where the factor $\eta_{i,m}$ represents the efficiency of the ptx or liquefaction system, i.e., the ratio of fuel output to electricity input. This equation holds also for methanation and Fischer-Tropsch systems, as they are modeled as integrated systems with integrated efficiencies (see discussion in Appendix D.2). Equation (10) together with Equation (2) then defines the link between the electricity market module and the energy transformation module, integrating the endogenous electricity demand. Short-term drops in the electricity price, for example, may cause ptx systems to ramp up their production and, in turn, their electricity demand. On the other hand, deep decarbonization of sectors, e.g., the road transport sector, may drive the demand for ptx fuels upwards, increasing electricity consumption. Greater electricity sector and, therefore, driving the endogenous electricity price upwards.

Analogous to the endogenous electricity price, the endogenous ptx fuel price represents another key link, which is implicitly visible to all modules as they are subject to one common cost-minimizing objective function. More specifically, for every unit of increased ptx fuel consumption in country m or export to another country, an additional unit of ptx fuel has to be produced in country m or imported from another country or from outside of Europe. The resulting increase in total system costs can be understood as the marginal price of that unit of additional fuel production. Thus, the endogenous market-specific ptx fuel price can be derived from the dual variables of the equilibrium conditions (7), (8) and (9) and represents the change in total system costs for supplying one more unit of ptx fuel.

Another key link between the energy transformation module and the electricity market and road transport modules is the endogenous ptx fuel demanded by the electricity and road transport sectors, defined via the energy consumption $\mathbf{ec}_{f,f1,m,s,t}$ for f1 = ptx fuels as part of the ptx fuel equilibrium conditions (7), (8) and (9). As such, the model has the option to decarbonize the electricity and road transport sectors using, e.g., a carbon-neutral ptx methane gas or a low-carbon natural gas and ptx hydrogen gas mix.

2.3. Simulating the European Road Transport Sector

A key contribution of this analysis lies within the detailed modeling of the European road transport sector and the representation of interlinkages with the electricity market and energy transformation modules. The road transport module invests in vehicle technologies as well as infrastructure to cover an exogenous demand for road transport. The choice of vehicle technology, in turn, drives the fuel demand for the road transport sector, being supplied by the electricity market module and the energy transformation module. In the following, the relevant parameters and assumptions (Section 2.3.1) as well as equations (Section 2.3.2) are presented in detail. Furthermore, the key variables and equations linking the road transport module to the electricity market and the energy transformation module are presented (Section 2.3.3).

2.3.1. Vehicle segments, vehicle technologies, fuels and infrastructure

Modeling the European road transport sector requires a detailed dataset to define parameters, which are categorized according to those that vary across vehicle segment, vehicle technology and fuel type.

The road transport sector is divided into three vehicle segments: private passenger vehicles (PPV), light-duty vehicles (LDV) and heavy-duty vehicles (HDV).²⁸ Similar to the approach for the electricity sector, technologies are defined for each of these vehicle segments; however, in the case of road transport, technologies can be understood as motor types. The vehicle technologies considered include gasoline motors, gasoline hybrids, diesel motors, diesel hybrids, natural gas motors, natural gas hybrids, battery electric vehicles (BEVs) and fuel-cell electric vehicles (FCVs). Hybrid vehicles (gasoline, diesel, natural gas) are represented by mild hybrids (HEVs) and plug-in hybrids (PHEVs). The existing technology mix in each country for 2015 as well as any recent growth in, e.g., electric vehicles between 2015 and 2017 is defined exogenously.²⁹ PPVs and LDVs are available for any fuel in Table 1 except for liquefied natural gas and liquefied hydrogen, which can solely be consumed by HDVs. HDVs have a variety of liquid fuels available, although gasoline is not assumed to be an option for heavy transport. Similarly, gaseous fuels such as hydrogen and gas are not available for HDVs in the road transport module due to lower energy densities and, as such, lower driving range (DLR et al. (2010), Bünger et al. (2016)).

As in the electricity market module, vintage classes are defined for each vehicle technology such that new investment objects are made available in future years to account for, e.g., cost degressions and technological innovations. One key cost component for vehicles is the investment cost or purchase price, with the values

 $^{^{28}}$ Light-duty vehicles are considered to weight less than 3.5 tonnes, heavy-duty vehicles more than 3.5 tonnes. Motorbikes, scooters and bicycles are excluded from this analysis, as are buses.

²⁹Based on European Commission (2016a), KBA (2017), IEA (2016a), CBS (2015), Statistics Sweden (2017), Statistics Norway (2017), Bundesamt für Statistik (2017), ZSW (2017) and Department of Transport (2017).

for PPVs, LDVs and HDVs shown in Tables D.8 - D.10 in Appendix D. The costs of vehicle technologies vary greatly not only according to the motor type but also across vehicle segments. This also holds true for fuel consumption, with values differing not only between, e.g., a diesel vehicle and a FCV but also between a passenger vehicle and a heavy-duty vehicle (see Tables D.14 - D.16 in Appendix D). As a result, under a sector-specific decarbonization target for the road transport sector, different vehicle technologies will compete not only within their segment (e.g., diesel PPV vs. FCV PPV) but also against the CO_2 abatement costs of the other segments (e.g., FCV PPV vs. FCV HDV).

In addition to investments in vehicle technologies, the model also endogenously builds the accompanying refueling or charging station infrastructure, depending on the fuel type. Just as in the other modules, infrastructure is an investment object with capital, FOM and variable costs.³⁰ Apart from refueling and charging station infrastructure costs, the distribution costs to the refueling or charging station is also taken into account and shown in Table D.17 in Appendix D.

As explained in Section 2.1.4, substitute fuels are defined as subsets to the fuel types and are priced according to how they were produced. Fossil-based hydrogen, CNG, LNG, gasoline and diesel as well as biogas, bio LNG, biogasoline and biodiesel are assumed to be available at global market prices. The fuel costs reflect not only the raw fuel prices but also additional production costs such as, e.g., natural gas reformation and oil refining. The price for electricity-based fuels, e.g. ptx gas, ptx diesel, etc., as well as the electricity price for BEVs and PHEVs are endogenously determined together with the electricity market and energy transformation modules.

2.3.2. Key aspects of modeling road transport and its infrastructure

The road transport module invests in vehicle technologies as well as infrastructure to cover an exogenous demand for road transport. The underlying equilibrium condition requires the exogenous demand road transport $dr_{m,t}$ to be covered by supply road transport $\mathbf{sr}_{i,m,t}$ summed over all vehicle technologies $i \in \mathbf{I_{rt}}$:

$$dr_{m,t} = \sum_{i} \mathbf{sr}_{i,m,t} \qquad \forall m,t.$$
(11)

The demand for road transport $dr_{m,t}$ defines the annual kilometers driven within each vehicle segment in each country up to 2050 (Tables D.11 - D.13 in Appendix D). Investments in vehicle technologies therefore supply the kilometers $\mathbf{sr}_{i,m,t}$ needed to serve demand based on a vehicle's annual driving distance, assumed to

³⁰Any additions or reinforcements to the electricity grid are not considered in this analysis.

be 13'800 km for PPVs, 21'800 km for LDVs and 70'000 km for HDVs.³¹ A single FCV PPV, for example, can supply 13'800 km of zero-carbon driving to a country's yearly demand for road transport. Large differences in yearly driving distance affect the vehicle lifetime, assumed to be 15 years for PPVs and 10 years for LDVs and HDVs. Such characteristics may influence the results as technologies in one vehicle segment must be replaced more often than others (e.g., FCV HDV vs. FCV PPV). In order to prevent a single technology from dominating the market from one time period to the next, maximum yearly adoption rates are defined, limiting the share of new registrations in the vehicle fleet in a single time period.³²

Carbon emissions and emission reductions in the road transport sector are accounted for as described in Section 2.1.5. Thereby, both direct and upstream emissions are accounted for via the decarbonization constraint (6), which also applies to the road transport sector.³³

2.3.3. Linking the road transport module to the electricity market and energy transformation modules

The fuel demanded, or energy consumed, by the road transport sector is determined endogenously based on the cost-optimal vehicle and infrastructure investments to cover the total demand for road transport per vehicle segment. The energy consumption $\mathbf{ec}_{f,f1,m,s,t}$ by fuel type f for the road transport sector s = rt is determined by the sum over supply road transport divided by the vehicle efficiencies $\eta_{i,m}$ for all vehicles iof the respective fuel type:

$$\sum_{f1} \mathbf{ec}_{f,f1,m,s,t} \bigg|_{s=rt} = \sum_{i} \mathbf{sr}_{i,m,t} / \eta_{i,m} \qquad \forall m, t, f,$$
(12)

with vehicle efficiency $\eta_{i,m}$ being the inverse of vehicle fuel consumption and $i \in \mathbf{I}_{rt}$.

One key link between the road transport module and the electricity market module is the direct use of electricity as a fuel for electric vehicles, i.e. PHEVs and BEVs. Combining Equations (12) and (2) is how the endogenous electricity demanded by electric vehicles, $\mathbf{ec}_{f,f1,m,s,t}$ for f1 = f = electricity, is accounted for in the electricity market module.³⁴ The endogenous electricity price represents another key link.

³¹Assumptions on annual driving distance and vehicle lifetimes are based on EWI et al. (2014), European Commission (2016a), McKinsey (2010), KBA (2017), Rhenus Logistics (2007), Knörr et al. (2012) and Papadimitriou et al. (2013).

 $^{^{32}}$ The upper bounds for the short term are taken from current data on new vehicle registrations and vary between 1.8% and 4.8% per year for a single vehicle technology. For the long term, they are assumed to increase up to 6.6%. The values are the same across vehicle technologies but vary across vehicle segments due to discrepancies between segment fleet sizes. These maximum adoption rates were set in order to best allow for an exponential deployment curve for new technologies. Note that the condition may become binding under strict decarbonization targets.

 $^{^{33}}$ Literature on the road transport sector often uses the concept of well-to-tank (WTT), i.e., the carbon emissions released during fuel production, and tank-to-wheel (TTW) emissions, i.e., the carbon emissions released upon combustion in the vehicle. In this analysis, the fuel-specific upstream carbon emission factor $\kappa_{f1,upstream}$ is analogous to the WTT emission factor in the road transport sector, whereas the fuel-specific carbon emission factor κ_{f1} is analogous to the TTW emission factor from vehicles. The road transport module therefore follows an approach, which is equivalent to a well-to-wheel (WTW) approach.

 $^{^{34}}$ For electric vehicles, exogenous hourly charging profiles are applied. Three types of charging stations are simulated: private

The key links between the road transport module and the energy transformation module are represented by the endogenous ptx fuel price and the ptx fuel demand of the road transport sector, i.e. its energy consumption $\mathbf{ec}_{f,f1,m,s,t}$ for f1 = ptx fuels, as defined in Equation (12), which directly feeds in the ptx fuel equilibrium conditions (7), (8) and (9). For example, under increased decarbonization targets, one option to decarbonize may be to displace carbon-heavy fossil fuels with ptx fuels. The increase in electricity consumption due to ptx fuel production is then accounted for via the energy transformation module and the electricity market module.

3. Application of the integrated model

In order to demonstrate the capabilities of the integrated model developed, an exemplary single scenario analysis is performed. The goal is to simulate the future European electricity-, road transport- and ptx-technology mix under sector-specific decarbonization targets and examine the role of electricity in achieving emission reductions. Within this section, first the scenario framework is presented (Section 3.1), followed by key results for the road transport sector (Section 3.2). The section ends with a discussion on the production of ptx fuels and how equilibrium is reached via the trading of ptx fuels throughout Europe (Section 3.3). The results for the European electricity sector are shown in Appendix F.

3.1. Scenario framework

The scenario is built on the medium- and long-term CO_2 targets given in the EU's climate strategy (European Commission (2014)). In the electricity market module, a sector-specific European emission reduction target is set to require a decline in emissions by 43 % compared to 2005 by 2030 and 90 % compared to 1990 by 2050. No additional national decarbonization targets for the electricity sectors are introduced. For the road transport sector, the decarbonization targets are set nationally, based on the Effort Sharing Decision of the European Commission for 2030 (European Commission (2016b)), shown in Table E.18 of Appendix E. The targets for 2050 converge to a 90 % emission reduction compared to 1990, consistent with the electricity sector target.³⁵ In addition to CO_2 constraints, the modeled scenario inhibits the energy transformation module from importing ptx fuels from outside of Europe.³⁶ The fuel price assumptions for

⁽e.g., households), semi-private (e.g., workplace) and public (fast charging). Private charging is assumed to take place mostly during evenings, whereas semi-public charging occurs primarily in daytime hours on weekdays. Public charging is possible at any hour but assumed to be less common than private and semi-private charging options (see, e.g., BAST (2015) and DLR (2015)). PHEV are assumed to follow the same charging profiles; however, PPVs are assumed to run 67% and LDVs 50% electric (see Kelly et al. (2012)).

 $^{^{35}}$ See Appendix E for a detailed description of the CO₂ target definition.

³⁶The goal of the analysis is to maximize the endogeneity of the model. Any exogenous decarbonization options such as ptx fuel imports from outside EU at fixed import costs may weaken the effects of the endgenous model output. Therefore, only endogenous investments in ptx and liquefaction capacities within Europe are allowed.

the scenario are based on a global commodity market at a price reflecting both the raw fuel and the fuel production costs (Figure E.2 in Appendix E). All other parameters are defined as described in Section 2.

3.2. Scenario results for the European road transport sector

The vehicle mix cumulated over all European countries is shown in Figure 3. The introduction of a country-specific sectoral decarbonization target in road transport drives an almost immediate alteration to the current vehicle mix. Hybrid (HEV) gasoline and diesel engines emerge as a short-term option to replace their fully internal combustion-powered counterparts. Furthermore, vehicles running on natural gas and electricity also show accelerated growth, with varying penetration levels across segments.



Figure 3: EU vehicle mix up to 2050 for PPVs (top left), LDVs (top right), HDVs (bottom left) and all vehicles (bottom right)

For the PPV segment, a mix of hybrid and internal combustion-powered vehicles running on compressed natural gas (CNG) dominate new vehicle investments in the short term. Starting in 2035, the model begins to maximize BEV deployment alongside continued investments in natural gas hybrids. HDVs also use natural gas to jump-start decarbonization, introducing internal combustion-powered trucks in 2020 and hybrid trucks in 2030 that run on liquefied natural gas (LNG) to push out their diesel counterpart; however, diesel HEVs remain in the vehicle mix through 2050. It is not until after 2040 that electric vehicles also begin to break through in the HDV segment, growing quickly to a 25% share of HDVs by 2050. LDVs, on the other hand, begin to maximize the deployment of electric vehicles early on, reaching upper bound adoption rates already in 2025. Natural gas LDVs help the remaining share to decarbonize, first via internal combustion-powered vehicles and then via plug-in hybrids. Hydrogen FCVs emerge in the LDV segment in 2045 and in the PPV and HDV segments in 2050, as the CO₂ bound becomes more and more restrictive.

Figure 4 provides further information about the fuel type consumed by the road transport sector.³⁷ The amount of fossil gasoline and diesel consumed in the road transport sector decreases by 46 % and 60 %, respectively, between 2020 and 2030. Within this decade, the amount of fossil CNG and LNG, on the other hand, increases ten-fold to account for over 40 % of all fuels consumed in 2030. As the techno-economic characteristics of the vehicles do not drastically differ from one another, the switch from gasoline and diesel to natural gas is driven primarily by comparatively lower well-to-wheel CO₂ emissions as well as cheaper fuel prices. The reduction in non-hybrid gasoline and diesel engines as well as gains in vehicle efficiency drive the total fuel consumption downwards.



Figure 4: Fuel consumption in the road transport sector in Europe in 2020, 2030 and 2050 in the coupled model

Non-fossil fuels mostly enter the market between 2030 and 2050 as a result of the long-term countryand sector-specific 90 % CO₂ reduction targets. Most notable is the increase in electricity, accounting for 570 TWh or 37 % of total fuel consumption in the European road transport sector in 2050. Restrictions in new vehicle deployment via maximum adoption rates are binding for BEVs in the PPV and LDV segments

 $^{^{37}}$ The results for the infrastructure follow the developments shown in Figure 4, as investments in infrastructure are made independent of vehicle segment and instead serve the total vehicle demand according to fuel type. A detailed discussion of the infrastructure results is omitted from this study as the focus lies primarily on the interdependencies between the modules rather than the individual module results.

relatively early on, which constrains the amount of electricity that can be directly consumed. As such, in order to reach the decarbonization targets, other low-carbon fuels must play a role. In particular, ptx fuels emerge from 2040 onwards, primarily for use in the HDV segment: First as liquefied gas mix and then together with ptx liquefied hydrogen (PtX LH2) and ptx diesel.³⁸ In fact, in 2050, over 55% of ptx fuels sold to the European road transport sector is consumed by HDVs. The remaining ptx fuels are in the form of ptx hydrogen gas (PtX H2) and ptx gasoline, consumed by the PPV and LDV segments. In total, the fuel share of ptx fuels in the European road transport sector reaches 27% by 2050. At this point, fossil as well as biogasoline and biodiesel are completely excluded from the fuel mix. Biogas, on the other hand, makes up a 20% share of total energy use.

Table F.19 of Appendix F shows the corresponding marginal CO_2 abatement costs for the road transport sector in each country for each model year. The countries with higher road transport demand and stricter CO_2 reduction targets in 2030 exhibit non-zero marginal CO_2 abatement costs in all years. A handful of other countries, however, appear to have zero costs for CO_2 abatement in several years up to 2040, i.e., the investments in lower-carbon vehicles and/or fuels are cost-efficient without any price signal from a binding CO_2 constraint. This holds particularly true for countries with higher shares of PPV and LDV demand, as the short-term switch to natural gas and electric cars/vans is cost competitive and thus appears to displace enough carbon emissions to undercut the decarbonization targets. Countries with higher shares of HDV demand, like Belgium, Poland and Spain, reveal some of the highest marginal CO_2 abatement costs in 2040 due to the consumption of liquefied gas mix, which is necessary to reach their sectoral decarbonization target. Because trucks have a higher fuel consumption and longer annual driving distance, the HDV segment in these countries is responsible for a larger share of the emissions. By switching from fossil LNG to low-carbon liquefied gas mix, the model can significantly reduce emissions without a major reinvestment in new vehicle technologies but rather maintaining (and adding to) the existing LNG and LNG hybrid HDV fleet.

By 2050, the country-specific marginal CO_2 abatement costs in the road transport sector in every country reach levels around 500 EUR/tCO₂ as the European-wide production and consumption of ptx fuels in all segments, especially the HDV segment, becomes necessary to reach the 90% reduction target. Investments in FCV HDVs (with ptx liquefied hydrogen) and BEV HDVs as well as FCVs (with ptx hydrogen gas) in the PPV and LDV segments in 2050 also add to the comparatively high marginal CO₂ abatement costs of the road transport sector.

 $^{^{38}}$ The striped areas in Figure 4 indicate the share of the gas mix that is decarbonized by ptx hydrogen gas. For example, in 2050, the liquefied gas mix consists of a share of 140 TWh that is decarbonized via ptx hydrogen gas feed-in (red striped area) and a share of 140 TWh liquefied natural gas (red area). For the years without any striped areas, the gas mix is completely fossil. For more information on the assumptions underlying the concept of gas mix, see Appendix D.2.

3.3. Supplying ptx fuels in an integrated modeling framework

Decarbonization of the road transport sector appears to create a demand for ptx fuels that must be supplied by either the countries themselves or imported from another European country. As such, a country's electricity market conditions (e.g., endogenous electricity demand, electricity generation mix, NTC constraints) as well as ptx fuel production conditions (e.g., endogenous electricity price, natural gas grid capacities, ptx fuel transport costs) will affect not only how their own road transport sector is decarbonized but whether they supply ptx fuels to or demand ptx fuels from other countries.

A deeper analysis of the ptx investment behavior provides insight into the cost-minimal supply of ptx fuels. Figure F.5 in Appendix F shows the development of ptx installed capacities and production across Europe between 2030 and 2050. As can be seen in the figure, investments in ptx first begin to take hold in 2040, with 22 GW electrolysis systems and 400 MW natural gas liquefaction plants. The hydrogen produced from the electrolysis systems (60 TWh) is completely fed into the natural gas grid to produce a low-carbon gas mixture, which is then liquefied (Liq. Gas Mix). The demand for liquefied gas mix in 2040 is driven by the need to decarbonize the fuel consumption in Belgium, Poland and Spain – the three countries with the highest share of HDVs. These three countries both consume their own gas mix production as well as import additional gas mix (via the natural gas grid) and liquefied gas mix (via tankers) to cover their ptx fuel demand. The two largest exporters of gas mix are France and Great Britain, who continue to have significant amounts of nuclear generation in 2040 next to large amounts of VRE. In addition, along with the third largest exporter Germany, these countries profit from large natural gas grid capacities available to feed-in ptx hydrogen gas as well as low transport costs due to the close proximity to the importing countries.

By 2050, the decarbonization targets in the road transport sector have driven every European country to both produce as well as consume ptx fuels. As shown in Figure F.5 in Appendix F, 114 GW_{el} of electrolysis systems and $3 \,\text{GW}_{el}$ of hydrogen and natural gas liquefaction plants are installed across Europe to produce hydrogen gas that is directly consumed (161 TWh_{th}), directly liquefied (56 TWh_{th}) or fed into the natural gas grid (140 TWh_{th}) and eventually liquefied. In addition, 12 GW_{el} of integrated electrolysis/Fischer-Tropsch systems are installed to produce ptx gasoline (16 TWh_{th}) and ptx diesel (33 TWh_{th}).

The ptx-fuel flows in 2050 are shown in Figure 5, with red indicating exporting countries and blue importing countries. In addition, Table F.20 in Appendix F provides key country-level results for 2040 and 2050 including the marginal costs of electricity generation as well as the average input electricity price for the electrolysis and integrated Fischer-Tropsch systems.³⁹

³⁹The average input electricity price is calculated for each ptx technology by summing the marginal costs of electricity

The map on the left-hand side shows the trading of gas mix, i.e., ptx hydrogen gas mixed into the natural gas grid. Although Poland has significantly lower marginal costs of electricity generation than Italy in 2050, the lack of sufficient natural gas grid capacity combined with growing pressure to reduce emissions from its HDV segment result in large import volumes of gas mix. Investing in methanation systems locally, which would be a possible alternative to trading gas mix, does not appear in the cost-optimal solution due to the lower methanation efficiency and resulting higher costs. The model maximizes the feeding-in of ptx hydrogen into the natural gas grid, and, as such, reaches the hydrogen feed-in limit for gas mix in Europe.



Figure 5: Net imports and exports of gas mix (left), ptx liquefied hydrogen (middle) and ptx diesel (right) in TWh_{th} , with positive values in blue indicating net import and negative values in red indicating net export

As a result, more fuels and/or vehicle technologies to reduce emissions are required to reach the sectorspecific decarbonization targets. With the maximum adoption rates for all BEVs, including the HDV segment, have been reached by 2050, the next cost-optimal decarbonization option that emerges in the road transport sector is the consumption of ptx liquefied hydrogen in fuel-cell trucks (FCV HDVs). In fact, all countries invest in FCV HDVs up to their maximum adoption rates during the five-year period between 2045 and 2050, creating a European-wide demand for ptx LH2. As shown in the middle map of Figure 5, several countries import significant (>1 TWh_{th}) amounts of ptx LH2 including Czech Republic, Germany, Great Britain, Italy and Poland. The three major exporters include Romania, Sweden and Finland, who not only have significant levels of VRE generation but nuclear generation as well. These effects drive the

generation across all hours in which the ptx system produces fuel and then dividing by the respective number of hours. By definition, an average input electricity price only exists if the ptx system is in operation.

marginal costs of electricity generation in these countries downwards, lowering the average electricity input price of ptx hydrogen production to 33, 21 and 14 EUR/MWh, respectively (Table F.20). The liquefaction of hydrogen, in particular, is an energy-intensive process and, as such, requires a large number of hours with very low electricity prices in order to be profitable. Despite the additional costs of transporting LH2, the exporting countries are able to supply the importing countries with ptx LH2 at lower cost than the countries would pay in producing the fuel themselves.

Binding adoption rates also for FCV HDVs however drive the need for an additional decarbonized fuel to enter the market, namely ptx diesel. Analogous to ptx LH2, ptx diesel is produced in select countries with profitable ptx conditions and then exported throughout Europe. The right-hand side of Figure 5 shows the corresponding trade flows. Fischer-Tropsch synthesis is, compared to electrolysis, significantly less efficient and, therefore, is only exported by the four countries with the lowest marginal electricity generation costs: Portugal, Sweden, Romania and Finland. As shown in Table F.20 in Appendix F, the Fischer-Tropsch systems in these countries have an average input electricity price ranging from 47-54 EUR/MWh, similar to their marginal costs of electricity generation. The greatest importer is Spain, who imports over 90% of its ptx diesel consumption (12 TWh_{th}) from Portugal in order to decarbonize its large HDV fleet. The other producers export small amounts of ptx diesel to fourteen countries across Europe.

Lastly, having exhausted the cost-optimal decarbonization options for the HDV segment, the model chooses to supply the PPV and LDV segments with ptx hydrogen gas by ramping up investments in fuel-cell vehicles in all countries. Convergence in decarbonization targets to 90 % reduction and similar price-setting abatement technologies result in converging marginal CO_2 abatement costs for the road transport sectors in 2050, as shown in Table F.19 in Appendix F. Due to very high transport costs of gaseous hydrogen, however, no trading of ptx hydrogen takes place. In other words, all countries supply and consume their own ptx hydrogen, despite significant differences in ptx production costs across countries. The share of ptx hydrogen of total fuel consumption ranges from 3% (Germany) to 20% (Ireland); however the maximum adoption rates are never reached. As a by-product of Fischer-Tropsch synthesis, the four exporters of ptx diesel also export small amounts of ptx gasoline for the PPV segments to the neighboring countries with the lowest transport costs, i.e., Spain, Bulgaria, Norway and Denmark.⁴⁰

 $^{^{40}}$ Fischer-Tropsch systems produce a wax (hydrocarbon mixture) that can be upgraded into different fuels. Within the scope of this study, it is assumed that for every unit of ptx diesel, nearly one half unit of ptx gasoline is produced (Becker et al. (2012)). See Appendix D.2 for more information.

4. Understanding the value of integrated models

Developing and applying an integrated model of this kind can be complex, requiring long computation times and intensive evaluation of the results and their implications. It is not uncommon to question whether such models are more valuable than single-sector or decoupled multi-sectoral models. The model created in this study addresses fundamental economic questions that, given a single market or multiple decoupled markets, could possibly be solved with, e.g., an analytical model. Yet the introduction of multiple coupled markets with integrated demands, substitute fuels across different fuel types, endogenous prices as well as trade possibilities requires that computer-based methods such as linear programming be used to account for the complexity of the coupling of the electricity sector to other sectors.

To provide a quantitative inclination of the added value of the integrated multi-sectoral model at hand, in the following, the results of the integrated model are compared to the results of a model run in which the modules are decoupled and the single sectors optimized independently of one another. In the decoupled model, all endogenous links between the modules are instead fed into the model exogenously. The logic and assumptions behind the exogenous parameters are explained in Section 4.1. The results are then compared to the coupled model in Section 4.2, with particular focus on key indicators such as CO_2 and electricity prices.

4.1. Decoupled versus coupled modules

In order to decouple the model, the endogenous links between the electricity market, road transport and energy transformation modules, i.e. the endogenous demands for electricity and ptx fuels, are broken such that each module stands on its own with its own exogenous inputs. As a result, the electricity market module invests in the cost-minimal electricity generation mix in order to cover its own demand, ignoring any additional electricity demand from electric vehicles or ptx technologies, just as in the original DIMENSION model. The road transport module can, nevertheless, invest in electric vehicles, resulting in an electricity demand; however, analogous to the fossil fuels, the module buys the electricity at an exogenous price.⁴¹ The energy transformation module is shut off in order for the electricity and road transport sectors to be independent of one another. Ptx fuels can, however, be bought by the electricity and road transport sectors at an exogenous price, just as is the case with supplying electric vehicles.⁴² Gas mix and liquefied gas mix,

 $^{^{41}}$ In this analysis, the exogenous electricity price is based on the LCOE of onshore wind generation, accounting for decreasing capital costs and technological improvements (see Figure G.6 in Appendix G). 42 The price for ptx fuels is determined according to the production costs, taking into account the annualized investment,

 $^{^{42}}$ The price for ptx fuels is determined according to the production costs, taking into account the annualized investment, variable and fixed costs of different ptx technologies. The electricity price assumptions for the ptx processes are – as for electric vehicles – based on the LCOE of onshore wind. The lack of endogenous information means that the ptx technologies can no longer optimize their electricity consumption according to hourly changes in the electricity price.

the result of feeding ptx hydrogen gas into the grid, is not considered in the decoupled case because the link between hydrogen production and gas mix demand cannot be quantified without the energy transformation module. Furthermore, no trading occurs as there is one single European market price for ptx fuels assumed. The exogenous ptx fuel prices as well as the exogenous electricity price for the road transport sector are shown in Figure G.6 in Appendix G.

4.2. Identifying the added value of integrated sector-coupled models

Figure 6 depicts the European electricity demand and electricity generation mix for the coupled and decoupled models in 2050 as well as the developments in marginal electricity generation costs and marginal CO_2 abatement costs in the electricity sector across Europe up to 2050. As expected, the electricity generation levels in the decoupled case are significantly lower (1300 TWh) than in the coupled case, as the additional electricity demand from the road transport and energy transformation modules (1200 TWh), indicated by the striped columns, and additional storage demand (100 TWh) is not accounted for.⁴³ The increase in electricity generation for the additional demand in the coupled model is mainly based on onshore wind and PV due to the identical decarbonization constraint.



Figure 6: Electricity demand by module and electricity generation by fuel type in Europe in 2050 for the coupled and decoupled model (left); Results of average European marginal electricity generation costs and marginal CO_2 abatement costs for the electricity sector in the coupled and decoupled model, including the exogenous electricity price used by the decoupled road transport and energy transformation modules (right)

The prices on the right side of Figure 6 also reflect these developments, with the dashed lines indicating the values from the decoupled model. Because the modules are optimized independently of one another, the

⁴³Any discrepancy between generation and demand in Figure 6 is due to transmission losses.

endogenous electricity price in the decoupled case only reflects the cost of supplying the demand within the electricity market module. While the difference in marginal electricity generation costs is negligible until 2030 due to limited demand increase, from 2040 onwards, the additional electricity demand from the road transport and energy transformation module results in higher marginal electricity generation costs. This is mainly due to fixed decarbonization targets subject to an increasing electricity generation. In 2050, the marginal electricity generation cost delta between the decoupled and coupled model is 16 EUR/MWh on average across all EU countries. The exogenous electricity price assumption for the road transport sector and the ptx fuel production, being based on the LCOE of wind onshore, underestimates the endogenous marginal electricity generation costs of the coupled model by 5 EUR/MWh on average across Europe. Analogous to the marginal electricity generation costs, the marginal CO₂ abatement costs for the electricity sector also begin to diverge from 2030 onwards, reaching a difference of $6 \text{ EUR}/tCO_2$ when comparing the coupled to the decoupled model results.⁴⁴

Comparing the results for the road transport sector, both the vehicle technology mix as well as fuel consumption behavior varies, most notably in the trade-off between ptx and fossil fuels. The results for the coupled and decoupled model in 2040 and 2050 are shown in Figure 7. In both models, the adoption rates for BEVs reach their maximum yearly values in the long term, leading the direct electricity consumption to be almost identical in both the coupled and decoupled cases. The same holds true for FCV HDVs and PtX LH2 in 2050. Nevertheless, the rest of the fuels show significant discrepancies between the coupled and decoupled cases beginning in 2040. The lack of available gas mix in the decoupled case makes it more expensive to decarbonize LNG and, in turn, drives a decrease in LNG consumption. As such, compared to the coupled case, HDVs in 2040 are supplied by greater amounts of low-cost fossil diesel, which is then balanced out by a growth in biofuel consumption (biogasoline, biodiesel, biogas).

By 2050, carbon-neutral ptx liquid methane (PtX LCH4) displaces much of the fossil LNG at levels equivalent to the decarbonized share of the liquefied gas mix (Liq. Gas Mix (PtX H2)) in the coupled case. Similar to 2040, lower levels of LNG consumption drive higher levels of diesel consumption in the HDV segment, which are, by 2050, entirely made up of carbon-neutral ptx diesel. In the decoupled case, 80% of all fuel consumption in the HDV segment in 2050 is ptx fuels, compared to the coupled case with 60%. Given the 90% decarbonization target in 2050, the decoupled model reacts to the increased ptx fuel consumption in the HDV segment by avoiding investments in fuel-cell vehicles, driving a 97% reduction in

 $^{^{44}}$ As discussed in Appendix F.2, the marginal CO₂ abatement costs of the electricity sector sink to 2 EUR/tCO₂ in 2030. Because the model is designed as a social planner problem with perfect foresight, the model anticipates the long-term decarbonization targets with early-on investments in VRE due to limited yearly adoption rates, driving down the marginal CO₂ abatement costs in 2030.



Figure 7: Difference in the fuel consumption in the road transport sector in Europe in 2040 and 2050 between the decoupled and the coupled model

FCV PPVs and 50% reduction in FCV LDVs with an accordingly lower ptx hydrogen consumption.

In sum, the total amount of ptx fuel consumption in the road transport sector is 15 TWh_{th} lower in the decoupled case compared to the coupled case, a discrepancy which arises due to the overestimation of ptx fuel costs in the decoupled case. More specifically, the exogenous electricity price used in estimating the production costs of the ptx fuels is a constant value that does not react to hourly changes in electricity market conditions. In the coupled model, however, the ptx systems can reduce their production costs by consuming electricity at times of low marginal costs of electricity generation. In the coupled case, for example, electrolysis operators pay on average across Europe 38 EUR/MWh for their electricity input in 2050 — an average of 15 EUR/MWh less than the exogenous price assumed in the decoupled case (see Table F.20 in Appendix F). As a result, the production costs of ptx hydrogen are overestimated in the decoupled case. The average EU input electricity price for ptx diesel, on the other hand, only differs by 2 EUR/MWh, which yiels similar production costs for ptx diesel across models.

Furthermore, endogenous electricity consumption of the ptx systems yields a significant price spread between the production costs of ptx hydrogen and ptx diesel in the coupled case. The decoupled case, on the other hand, does not take the differences in electricity input prices across ptx systems into account and, as such, exhibits a smaller price spread between ptx hydrogen and ptx diesel. This change in ptx fuel price spreads drives a change in the merit order of decarbonization options: low-cost diesel hybrid (HEV) HDVs fueled with ptx diesel appears to jump ahead of high-cost fuel cell LDVs and PPVs fueled with ptx hydrogen in the decoupled model. Thus, in the decoupled model, decarbonization in the HDV segment is stronger, leaving room for reduced decarbonization in the PPV and LDV segments. The overestimation of ptx production costs and the accompanying change in investment behavior has a direct effect on the marginal CO_2 abatement costs of the road transport sector, with an overestimation of approximately 30 EUR/tCO_2 in the decoupled model (see Table G.21 in Appendix G).

Overall, the decoupled model overestimates the total system costs in 2050 by 30 billion EUR. The difference in total system costs is a result of the inaccuracy of the estimations for exogenous costs such as electricity and ptx fuel costs compared to the endogenous system costs resulting from the integrated model. In particular, the overestimation of electricity input costs for ptx systems due to a disregard of their flexibility potential adds to the increase in total system costs of the decoupled model.

5. Conclusion

This analysis introduces and assesses an integrated multi-sectoral partial-equilibrium investment and dispatch model to simulate the coupling of the European electricity and road transport sectors. The focus lies not only on depicting a detailed technological representation within each sector but also on properly accounting for any interconnections resulting from electricity consumption from electric mobility or from energy transformation via ptx processes. High technological, spatial and temporal granularity allows for the optimization of European electricity and ptx fuel production as well as the simulation of cost-minimizing trade flows according to endogenous market conditions.

The integrated multi-sectoral model is applied for an exemplary scenario to analyze the effects of sectorspecific CO_2 reduction targets (-90 % by 2050 compared to 1990) on the vehicle, electricity and ptx technology mix in European countries from 2020 to 2050. The results show that both electricity and ptx fuels play a key role in decarbonizing the road transport sector, reaching 37% and 27% of total fuel consumption in 2050, respectively. The HDV segment, in particular, demands the majority of ptx fuels in Europe, consuming liquefied gas mix, ptx liquefied hydrogen and ptx diesel that is produced primarily in high VRE countries such as Portugal and Sweden. Coupling of the electricity and road transport sectors results in 1200 TWh additional electricity demand in Europe, with average marginal costs of electricity generation across Europe reaching 58 EUR/MWh in 2050.

In order to understand the added value of building complex integrated models, the second part of the analysis examines an identical scenario with decoupled sectors, removing all endogenous ties between sectors and allowing each to be optimized independently of one another. Comparison between the two scenario results confirms that quantitative methods that fail to account for the interdependencies between the electricity and road transport sectors may significantly overestimate the total system costs. The flexibility of ptx systems, in particular, cannot be taken into account once exogenous annual electricity prices are used. As shown in the decoupled model results, ignoring fluctuations in short-term electricity prices may lead to the costs of ptx fuels to be falsely estimated, which may affect the merit order of decarbonization options under strict CO_2 reduction targets and thereby result in substantially different technology choices.

In future work, further detailed scenarios and sensitivity analyses could increase the understanding of the robustness of the presented decarbonization pathway. In particular, the effects of behavioral aspects regarding, e.g., the adoption of new technologies, driving patterns or consumer preferences could be investigated. Furthermore, endogenous charging of electric vehicles may be a promising extension. The model could also be extended to simulate additional modes of transport that may contribute to decarbonization such as, e.g., rail. Although excluded from the discussion, the modeling of the infrastructure for the road transport may be improved to include, e.g., electricity grid investments. Additionally, further research efforts could go into the refining of temporal resolution and technological granularity.

Appendix A. Nomenclature and abbreviations

Throughout the paper, notation as listed in Table A.1 is applied. Unless otherwise noted, bold capital letters indicate sets, lowercase letters parameters and bold lowercase letters optimization variables.

Sets		
$f \in \mathbf{F}$		Fuel type $(f1: \text{Subfuels})$
$i \in \mathbf{I}$		Technologies (electricity generators, ptx plants, cars)
$m,n\in\mathbf{M}$		Markets
$s \in \mathbf{S}$		Sector (rt: road transport, el: electricity, et: energy transformation)
$t \in \mathbf{T}$		Time (\mathbf{T} : time slices)
Parameters		
$l_{m,t}$	MWh	Exogenous electricity demand
l_{peak}	MWh	Peak electricity demand
$dr_{m,t}$	bn. km	Exogenous demand road transport
x	-	Availability of electricity generator
v	-	Capacity value of electricity generators
$ar{k}$	MW	Transmission capacity
η	-	Efficiency
δ	EUR/MW	Fixed costs
γ	EUR/MW	Variable costs electricity generation
κ_{f1}	tCO_2eq/MWh	Fuel-specific emission factor
$\kappa_{f1,upstream}$	tCO_2eq/MWh	Fuel-specific upstream emission factor
$GHG_{cap,s,t}$	tCO_2eq	Sector-specific greenhouse gas emissions cap
TC	bn. EUR	Total costs
Optimization variables		
x	MW	Electricity generation capacity
g	MWh	Electricity generation
k	MWh	Electricity transmission between markets
ec	MWh	Energy consumption
sr	bn. km	Supply road transport
\mathbf{fp}	MWh	Fuel production
\mathbf{ft}	MWh	Fuel trade
ffi	MWh	Fuel feed-in
em	tCO_2eq	GHG emissions
cpt	tCO_2	CO_2 capture

Table A.1: Model sets, parameters and variables

AT	Austria	FI	Finland	NL	Netherlands
BE	Belgium	\mathbf{FR}	France	NO	Norway
BG	Bulgaria	GB	Great Britain	PL	Poland
CH	Switzerland	\mathbf{GR}	Greece	\mathbf{PT}	Portugal
CZ	Czech Republic	\mathbf{HR}	Croatia	RO	Romania
DE	Germany	HU	Hungary	SE	Sweden
DK (East)	Eastern Denmark	IE	Ireland	\mathbf{SI}	Slovenia
DK (West)	Western Denmark	\mathbf{IT}	Italy	SK	Slovakia
EE	Estonia	LT	Lithuania		
\mathbf{ES}	Spain	LV	Latvia		

Table A.2: Country codes

a	Years
BEV	Battery electric vehicle
bn	Billion
CAES	Compressed air energy storage
CCU	Carbon capture and utilization
CHP	Combined heat and power
CHP	Open cycle gas turbine
CNG	Compressed natural gas
CO2	Carbon dioxide
cn	Compared to
CSP	Concentrated solar power
DAC	Direct air capture
DSB	Demand side response
El/ol	Electricity / electric
	Equivalent
FUR	Furo
FCV	Fuel cell vehicle
FON	Fixed operation and maintenance
CW	Circulation and maintenance
GW	Gigawatt
	nydrogen Weter
$\Pi_2 O$	Water
HDV	Heavy-duty venicle
HEV	Hybrid electric venicle
km	Kilometer
kW_{el} / kW_{th}	Kilowatt (electric / thermal)
kWh _{el} / kWh _{th}	Kilowatt hours (electric / thermal)
LCA	Life cycle analysis
LCOE	Levelized costs of electricity
LDV	Light-duty vehicle
LH2	Liquid hydrogen
Liq	Liquefaction/liquefied
LNG	Liquefied natural gas
m	Million
$MtCO_2$ eq	Million tons carbon dioxide equivalent
MW	Megawatt
NTC	Net transmission capacity
O_2	Oxygen
OCGT	Open-cycle gas turbine
PEM	Polymer electrolyte membrane electrolysis
PHEV	Plug-in hybrid electric vehicle
PPV	Private passenger vehicles
PtX	Power to X (heat, gas, liquid, fuel, chemicals etc.)
PtX H2	Ptx hydrogen gas
PtX LH2	Ptx liquid hydrogen
PtX CH4	Ptx methane gas
PtX LCH4	Ptx liquid methane
PV	Photovoltaics
$^{\mathrm{th}}$	Thermal
t	Ton
TTW	Tank-to-wheel
TW	Terawatt
VRE	Variable renewable energy
WTT	Well-to-tank
WTW	Well-to-wheel

Table A.3: Abbreviations

Appendix B. Modeling the European electricity sector

The model covers all 28 countries of the European Union, except for Cyprus and Malta, but includes Norway and Switzerland. Existing electricity generation capacities in 2015 are based on a detailed power plant database developed at the Institute of Energy Economics at the University of Cologne, which is mainly based on the Platts WEPP Database (Platts (2016)) and regularly updated. The investment decisions and generation profiles for a wide range of power plants are optimized endogenously. These include conventional, combined heat and power (CHP), nuclear, onshore and offshore wind turbines, roof and ground photovoltaic (PV) systems, biomass (CHP-) power plants (solid and gas), hydro power plants, geothermal power plants, concentrating solar power (CSP) plants and storage technologies (battery, pump, hydro and compressed air energy (CAES)).⁴⁵ Only countries without existing nuclear phase-out policies are allowed to invest in nuclear power plants. Investments in carbon capture and storage (CCS) technologies are not allowed due to a general lack of social acceptance in European countries. Technological improvements in, e.g., efficiency are taken into account using vintage classes. These are then included in the model as an additional technology option that is only available from a certain point in time onwards.

The objective function of the model seeks to minimize the accumulated discounted total system costs.⁴⁶ All cost assumptions for technologies listed above are taken from the power plant database at the Institute of Energy Economics at the University of Cologne. Key cost factors are investment, fixed operation and maintenance and variable production costs as well as costs due to ramping thermal power plants. Investment costs occur for new investments in generation and storage units and are annualized with a 7% interest rate for the depreciation time. The fixed operation and maintenance costs represent staff costs, insurance charges, interest rates and maintenance costs. Variable costs are determined by the fuel price, net efficiency and total generation of each technology. Depending on the ramping profile additional costs for attrition occur. CHP plants can generate income from the heating market, thus reducing the objective value (Jägemann et al. (2013)). The model applies a discount rate of 2.75% for discounting of future cashflows to the present (net present value).

Short-term deployment of renewable technologies is taken into account via minimal deployment targets (based on ENTSO-E (2015a)) for 2020 and remain constant up to 2050.⁴⁷

 $^{^{45}}$ The use of lignite and biomass sources (solid and gaseous) is restricted by a yearly primary energy potential in MWh per country.

⁴⁶The total system costs do not include investment costs for electricity grid extensions nor operational costs for grid management.

 $^{^{47}}$ This statement holds true for all technologies with the exception of offshore wind. Expected deployment projections were taken from WindEurope (2017) for 2020 and EWEA (2015) for 2030 and 2050

The model also considers several subregions within the countries, which differ with regard to the hourly electricity feed-in profiles and the achievable full load hours of wind turbines (onshore and offshore) and solar power plants (PV and CSP) per year. Overall, the model distinguishes between 47 onshore wind, 42 offshore wind and 38 solar subregions across Europe. The hourly electricity feed-in of wind and solar power plants per subregion are based on historical hourly wind speed and solar radiation data by EuroWind (2011).⁴⁸ The deployment of wind and solar power technologies is restricted by a space potential in km² per subregion.

Yearly national electricity consumption is assumed to follow the Ten-Year Network Development Plan (TYNDP) from ENTSO-E (2015b) and the European Commission's e-Highway 2050 Project (European Commission (2015)). It is important that the countries' future electricity consumption, i.e., their exogenous electricity demand, does not assume any additional electricity demand from, e.g., electric vehicles or power-to-x systems. This additional electricity demand is determined endogenously from the energy transformation and road transport modules. Therefore, specific scenarios fitting this criteria were chosen from ENTSO-E (2015b) and European Commission (2015), namely the Small & Local scenario for 2040 and 2050. Hourly electricity demand is based on historical hourly load data from ENTSO-E (ENTSO-E (2012)). Interconnector capacities are taken into account via one node per country. Hence, the model covers 28 countries connected by 65 transmission corridors. Existing and future extensions of net-transfer capacities are exogenously defined and may in some cases limit the power exchange across country borders. This data has been taken from ENTSO-E (2015b), Bundesnetzagentur (2016) and European Commission (2015).

 $^{^{48}}$ While the securely available capacity of dispatchable power plants within the peak-demand hour is assumed to correspond to the seasonal availability, the securely available capacity of wind power plants (onshore and offshore) within the peak-demand hour (capacity value or capacity credit) is assumed to amount to 5%. In contrast, PV systems are assumed to have a capacity value of 0% due to the assumption that peak demand occurs during evening hours in the winter. A peak-demand constraint ensures enough back-up capacity to meet security of supply requirements given a high share of fluctuating renewables (Jägemann et al. (2013)).

Appendix C. Key links between the modules

Figure C.1 provides an illustration of the links between the electricity market, the energy transformation and the road transport modules, represented by endogenous demands for electricity and ptx fuels as well as the respective endogenous prices resulting from the integrated optimization.



Figure C.1: Exchange of endogenous information between the modules in the integrated model

Appendix D. Additional data and assumptions

Substitute Fuel	$\begin{array}{c} {\bf Direct \ Emissions} \\ {{\left({{\bf TTW}} \right)}^{49}} \end{array}$	$\begin{array}{l} { { { Upstream \ Emis}} \\ { sions \ (WTT)}^{50} \end{array} \end{array}$	Description Production Cycle (plus dispensing at retail site)
Diesel	0.268	0.052	Crude oil production, crude refining. distribution
Biodiesel	0.268	0.192	Rape cultivation, rapeseed drying, oil production, biodiesel production, distribution
PtX Diesel	0.268	0.005	Distribution
Gasoline	0.253	0.046	Crude oil production, crude refining, distribution
Biogasoline	0.253	0.191	Wheat cultivation, grain drying, storage and han- dling, ethanol production, distribution
PtX Gasoline	0.253	0.005	Distribution
CNG	0.204	0.028	NG production, distribution, compression
Biogas (hc)	0.204	0.053	Fermentation, upgrading, compression, distribu- tion
Biogas (lc)	0.204	0.053	Fermentation, upgrading, compression, distribu- tion
PtX CH4	0.204	0.012	Distribution
LNG	0.204	0.053	NG production, lique faction, loading & unloading terminal, road transport
Bio LNG	0.204	0.077	Fermentation, upgrading, liquefaction, distribution
PtX LCH4	0.204	0.016	Distribution
H2	0.000	0.334	NG production, stream reforming, pipeline, compression
PtX H2	0.000	0.047	Distribution
LH2	0.000	0.423	NG production, stream reforming, liquefaction, road transport
PtX LH2	0.000	0.015	Distribution
Biosolid	0.327	0.028	Wood plantation & chipping
Coal	0.339	0.059	Hard coal provision
Lignite	0.403	0.020	Lignite provision
Nuclear	0.000	<0.001	Uranium ore extraction, fuel production

Appendix D.1. Direct and upstream emission factors

Table D.4: Direct and upstream emission factors [tCO₂eq/MWh]

⁵⁰ The upstream emission factors are taken from Edwards et al. (2014) and include CO₂ emissions resulting from production and conditioning. Any CO₂ emissions emitted during transportation of the fuel to market is not accounted for in the upstream emission factor.

 $^{^{50}}$ The direct emissions factors are taken from Department for Business, Energy and Industrial Strategy (2016) and UBA (2017).

Appendix D.2. Selected data and assumptions used in the energy transformation module

In the following, additional explanations and technical details about the technologies used in the energy transformation module are presented. An electrolysis system uses electricity in an endothermic process to split water into hydrogen and oxygen. Alkaline and PEM electrolysis vary according to their electrolyte solution and electrode composition; however, both operate at temperatures ranging from 50 to 80 degrees Celsius. The hydrogen produced can either be sold directly or be stored to successively produce methane via catalytic methanation, hydrocarbons via Fischer-Tropsch synthesis, or a low-carbon natural gas mixture via feeding into the natural gas grid. During catalytic methanation, carbon dioxide and hydrogen undergo an exothermic reaction at temperatures between 200 and 400 degrees Celsius to yield methane, steam and heat.⁵¹ Fischer-Tropsch synthesis is a more complex process in which carbon monoxide and hydrogen build carbon chains via a series of exothermic reactions followed by an endothermic hydrocracking isometrisation distillation to separate the crude product into usable fuels (e.g., ptx gasoline, ptx diesel). A simplified production ratio of ptx gasoline to ptx diesel of 9.8: 20.1 is applied in the model (Becker et al. (2012)). CO₂ is used to create the carbon monoxide via reverse CO shift (Schmidt et al. (2016)).

The feed-in of hydrogen into the natural gas grid is modeled with an upper limit of 10 vol-% of natural gas. Note that hereby it is assumed that the changes in the energy density of the gas mix (natural gas / ptx hydrogen gas mix) are negligible, i.e., one MWh of injected ptx hydrogen adds one MWh to the natural gas supply, or, stated differently, it substitutes one MWh of natural gas and thereby reduces the amount of CO₂ emissions from combustion accordingly. Thereby, the model implicitly assumes a certificate market for units of decarbonized gas (i.e., hydrogen feed-in). As such, the energy transformation module can feed-in hydrogen gas up the upper 10 vol-% limit, being based on the natural gas allows the road transport module to buy decarbonized gas. Note that thereby the total amount of decarbonized gas consumed in the road transport sector may exceed 10 vol-% of the total gas consumption of the road transport, as the feed-in limit is defined on total gas demand of all sectors and not of the road transport sector alone. In a model covering multiple sectors, the single sectors thereby compete for low-cost decarbonized gas via hydrogen feed-in on the certificate market.

For every mole of hydrogen produced, an electrolysis system produces a half-mole of oxygen that can be sold to, e.g. the industry or services sectors. The amount of oxygen produced is determined stoichiometrically

 $^{^{51}}$ As the heating sector is not accounted for in this analysis, efficiency gains due to the recycling of the heat generated by methanation is not considered.

based on the amount of ptx hydrogen produced by electrolysis, which is driven not only by the endogenous hydrogen demand but from the need for ptx hydrogen in the methanation or Fischer-Tropsch processes as well. To determine the amount of oxygen produced, octane was assumed for gasoline and hexadecane for diesel.

Table D.5 gives an overview of the key assumptions made for each ptx investment object considered in the energy transformation module with regard to investment costs, FOM costs, efficiency and technical lifetime. It should be noted that only integrated systems are considered for methanation and Fischer-Tropsch systems, meaning that all investments in methanation and Fischer-Tropsch technologies include the simultaneous investment in a PEM electrolysis to produce the ptx hydrogen required in the subsequent methanation or Fischer-Tropsch processes. Therefore, the techno-economical parameters, e.g., investment costs, for methanation and Fischer-Tropsch systems in Table D.5 are for integrated, as opposed to standalone, systems. This is especially important when considering the efficiencies, which are always defined with respect to the electricity input of the integrated system, i.e., the amount of fuel output relative to the amount of electricity input.⁵² The FOM costs also include the stack replacement costs of the electrolysis system, calculated based on the assumptions in Grahn (2017).

Conversion systems to liquefy gaseous hydrogen or natural gas are also taken into account in the energy transformation module. Because liquefaction plants also consume electricity, they are modeled analogous to ptx systems as investment objects. Unlike the integrated ptx systems, liquefaction plants are assumed to be stand-alone systems. The techno-economic assumptions for the liquefaction plants are in Table D.6.

 $^{^{52}\}mathrm{PEM}$ electrolysis in integrated systems is also allowed to produce ptx hydrogen in stand-alone mode.

		2020	2030	2050	Main sources
	Alkaline Electrolysis	833	500	383	Henning and Palzer (2015), FfE (2016), Elsner and Sauer (2015), Schiebahn et al. (2015)
[EUR/(kW el)]	PEM Electrolysis	980	545	484	Elsner and Sauer (2015), Schmidt et al. (2016)
	Methanation (coupled with a PEM electroly- sis)	1317	845	717	Grahn (2017), Brynolf et al. (2018), Tremel et al. (2015)
	Fischer-Tropsch (coupled with a PEM electrolysis)	1887	1152	917	Grahn (2017), Brynolf et al. (2018), Tremel et al. (2015), Smejkal et al. (2014)
	Alkaline Electrolysis	40	21	16	Schmidt et al. (2016), Grahn (2017)
FUM costs (including stack replacement costs	PEM Electrolysis	50	23	18	Schmidt et al. (2016), Grahn (2017)
for electrolysis) [EUR/(kW*a)]	Methanation (coupled with a PEM electroly- sis)	63	35	28	Schmidt et al. (2016), Grahn (2017)
	Fischer-Tropsch (coupled with a PEM electrolysis)	83	46	37	Schmidt et al. (2016), Grahn (2017)
- - - - -	Alkaline Electrolysis	0.67	0.70	0.70	FfE (2016), Elsner and Sauer (2015), Schiebahn et al. (2015)
Emciency [MWh th/MWh el]	PEM Electrolysis	0.65	0.67	0.71	Schmidt et al. (2016)
- 	Methanation (coupled with a PEM electroly- sis)	0.48	0.50	0.54	Schmidt et al. (2016), Grahn (2017), Brynolf et al. (2018), Tremel et al. (2015)
	Fischer-Tropsch (coupled with a PEM electrolysis)	0.45	0.47	0.51	Schmidt et al. (2016), Grahn (2017), Brynolf et al. (2018), Tremel et al. (2015)
	Alkaline Electrolysis	15	20	25	Henning and Palzer (2015), FfE (2016), Elsner and Sauer (2015), Schiebahn et al. (2015)
Technical Lifetime [a]	PEM Electrolysis	15	20	25	FfE (2016), Elsner and Sauer (2015), Schiebahn et al. (2015)
	Methanation (coupled with a PEM electroly- sis)	15	20	25	Elsner and Sauer (2015), Brynolf et al. (2018), Parra and Patel (2016)
	Fischer-Tropsch (coupled with a PEM electrolysis)	15	20	25	Brynolf et al. (2018), Becker et al. (2012)
Interest rate [%]	All	2	2	2	Kost et al. (2018)

Table D.5: PtX Cost

3.53 Amos (1998), Krewitt and Schmid (2005),U.S. Department of Energy (2009)	25 Krewitt and Schmid (2005)	$^{\prime}$ 761 $^{\prime}$ 622 Pfennig et al. (2017)	91 Krewitt and Schmid (2005)	7 Fraunhofer 2018	17.37 Franco and Casarosa (2014)	20 Schmidt et al. (2016)	5286 / 4927 Schmidt et al. (2016), Songhurst (2014)	211 Schmidt et al. (2016)	7 Kost et al. (2018)
${ m Efficiency}~({ m MWh_fuel}/{ m MWh_el})$	Technical Lifetime (a)	$ \begin{array}{cccc} {\rm Invest \ Costs \ 2020/2030/2050} & 1588 \\ {\rm (EUR/kW_el)} \end{array} \end{array} $	FOM Costs (EUR/kW_ el^*a)	Interest Rate $(\%)$	${ m Efficiency}~({ m MWh_fuel}/{ m MWh_el})$	Technical Lifetime (a)	Invest Costs 2020/2030/2050 5466 / (EUR/kW_el)	FOM Costs (EUR/kW_ el^*a)	Interest Rate (%)
Hvdroen	Liquefaction					Methane/	Natural Gas Liquefaction		

assumptions	
Liquefaction	
Table D.6:	

Fuel transport costs between markets [E	UR/MWh/km]
PtX Gasoline/PtX Diesel	0.010
Gas Mix/PtX CH4	0.002
Liq. Gas Mix/PtX LCH4	0.015
PtX H2	0.090
PtX LH2	0.020

Table D.7: Ptx fuel transport costs between markets 53

Appendix D.3. Selected data and assumptions used in the road transport module

In the following, additional details about the technologies used in the road transport module are presented.

	2015	2020	2030	2040	2050
Gasoline	22'475	22'573	22'769	22'769	22'769
Diesel	24'275	24'373	24'569	24'569	24'569
Gasoline HEV	23'890	23'752	23'476	23'123	22'769
Diesel HEV	25'803	25'646	25'332	24'951	24'569
Gasoline PHEV	31'774	30'125	26'829	26'110	25'371
Diesel PHEV	34'318	32'529	28'950	28'174	27'377
CNG	24'729	24'631	24'436	24'363	24'289
CNG HEV	26'286	25'922	25'195	24'742	24'289
CNG PHEV	34'960	32'905	28'793	27'979	27'146
H2 FCV	66'746	54'892	31'184	27'990	24'796
BEV	34'900	31'042	27'581	26'114	24'646

Table D.8: PPV Vehicle Cost [EUR/vehicle]⁵⁴

	2015	2020	2030	2040	2050
Diesel	26'003	26'585	27'748	27'748	27'748
Diesel HEV	31'156	30'966	30'498	29'123	27'748
Diesel PHEV	41'437	38'523	32'696	31'820	30'920
CNG	28'955	28'841	28'612	28'526	28'440
CNG HEV	34'692	33'594	31'448	29'940	28'440
CNG PHEV	46'141	41'999	33'714	32'761	31'785
\mathbf{BEV}	41'021	36'967	32'100	30'392	28'684
H2 FCV	78'452	64'519	36'653	32'899	29'145

Table D.9: LDV Vehicle Cost [EUR/vehicle]⁵⁵

⁵³Based on Balat (2008), Dodds and McDowall (2014), IEA (2013), Yang and Ogden (2007).

⁵⁴Own calculations based on Wietschel et al. (2010), Fraunhofer IWES et al. (2015), Henning and Palzer (2015), ADAC (2015), Arndt et al. (2016), IEA (2017) and Özdemir (2011).

⁵⁵Own calculations based on Wietschel et al. (2010), Fraunhofer IWES et al. (2015), Henning and Palzer (2015), ADAC (2015), Arndt et al. (2016), IEA (2017) and Özdemir (2011).

⁵⁶Own calculations based on Wietschel et al. (2010), Fraunhofer IWES et al. (2015), Henning and Palzer (2015), ADAC (2015), Arndt et al. (2016), IEA (2017) and Özdemir (2011).

	2015	2020	2030	2040	2050
Diesel	108'157	109'959	113'565	113'565	113'565
Diesel HEV	144'209	143'332	140'757	138'181	135'196
LNG	130'689	130'046	128'758	127'471	126'183
LNG HEV	174'253	170'819	163'952	157'085	150'218
BEV	441'640	397'219	250'000	180'000	130'689
LH2 FCV	441'640	397'219	308'376	219'533	130'689

Table D.10: HDV Vehicle Cost $\left[\mathrm{EUR/vehicle}\right]^{56}$

	2015	2020	2030	2040	2050
AT	65	67	71	76	80
\mathbf{BE}	76	82	89	95	101
BG	34	35	37	39	40
\mathbf{HR}	19	21	23	24	26
\mathbf{CZ}	48	52	60	68	75
DK (East)	16	17	18	18	19
DK (West)	18	20	21	22	22
EE	8	8	9	9	10
FI	48	48	50	51	52
\mathbf{FR}	453	480	507	533	550
\mathbf{DE}	621	626	651	663	671
\mathbf{GB}	417	444	483	513	540
\mathbf{GR}	58	59	60	62	63
HU	29	32	36	41	45
IE	31	34	41	45	48
\mathbf{IT}	342	358	379	387	407
\mathbf{LV}	9	10	10	11	11
\mathbf{LT}	17	18	19	19	20
\mathbf{NL}	104	108	114	120	125
NO	33	34	36	37	39
\mathbf{PL}	112	128	149	167	179
\mathbf{PT}	56	57	64	68	72
RO	42	46	57	67	74
\mathbf{SK}	14	17	22	24	26
SI	16	17	19	20	21
\mathbf{ES}	192	201	231	257	278
\mathbf{SE}	77	79	86	91	95
\mathbf{CH}	59	61	65	69	74

Table D.11: PPV Road Transport Demand [Billion $\mathrm{km}]^{57}$

	2015	2020	2030	2040	2050
\mathbf{AT}	11	12	14	16	18
\mathbf{BE}	13	14	16	17	19
BG	3	3	3	3	3
\mathbf{HR}	4	5	5	6	6
\mathbf{CZ}	9	9	11	12	13
DK (East)	5	5	6	7	8
DK (West)	6	6	6	7	8
\mathbf{EE}	1	1	1	1	1
FI	5	6	6	6	7
\mathbf{FR}	118	125	140	156	174
DE	44	46	51	57	62
GB	73	75	81	87	94
\mathbf{GR}	14	15	17	18	20
HU	9	9	10	11	12
IE	16	16	18	20	21
IT	85	87	92	96	101
LV	1	1	2	2	2
\mathbf{LT}	2	2	3	3	3
NL	21	22	23	25	28
NO	9	10	11	12	13
\mathbf{PL}	21	23	30	38	48
\mathbf{PT}	21	21	22	23	24
RO	7	7	8	9	10
SK	4	4	5	5	6
SI	3	3	4	4	E.
\mathbf{ES}	22	23	24	26	28
SE	12	12	13	14	15
CH	4	5	5	5	6

Table D.12: LDV Road Transport Demand [Billion km] ⁵

 $^{^{57}\}mathrm{Own}$ calculations based on European Commission (2016a) and EWI et al. (2014). $^{58}\mathrm{Own}$ calculations based on European Commission (2016a) and EWI et al. (2014).

	2015	2020	2030	2040	2050
AT	4	4	5	6	6
\mathbf{BE}	11	12	15	17	18
BG	1	1	1	2	2
\mathbf{HR}	1	1	2	2	2
\mathbf{CZ}	5	6	6	7	8
DK (East)	1	2	2	2	2
DK (West)	2	2	2	3	3
\mathbf{EE}	0	0	0	0	0
\mathbf{FI}	2	3	3	3	3
\mathbf{FR}	30	34	42	47	50
\mathbf{DE}	53	59	67	70	72
\mathbf{GB}	33	34	38	41	44
\mathbf{GR}	4	5	5	5	6
\mathbf{HU}	3	3	4	4	4
IE	1	2	2	3	3
\mathbf{IT}	20	22	24	26	28
\mathbf{LV}	1	1	1	1	1
\mathbf{LT}	1	1	1	1	1
\mathbf{NL}	7	8	8	9	9
NO	2	3	3	3	3
\mathbf{PL}	25	28	35	40	43
\mathbf{PT}	1	2	2	2	2
RO	3	4	5	6	6
\mathbf{SK}	2	2	3	3	3
\mathbf{SI}	1	1	2	2	2
\mathbf{ES}	51	55	63	70	75
\mathbf{SE}	3	3	3	4	4
\mathbf{CH}	4	5	5	5	6

Table D.13: HDV Road Transport Demand [Billion $\mathrm{km}]^{59}$

 $^{^{59}\}mathrm{Own}$ calculations based on European Commission (2016a) and EWI et al. (2014).

	2015	2020	2030	2040	2050
Gasoline	0.71	0.60	0.55	0.53	0.53
Diesel	0.66	0.54	0.46	0.42	0.42
Gasoline HEV	0.46	0.43	0.40	0.36	0.34
Diesel HEV	0.43	0.40	0.37	0.36	0.34
Gasoline PHEV	0.37	0.33	0.29	0.28	0.28
Diesel PHEV	0.35	0.31	0.26	0.24	0.24
CNG	0.70	0.61	0.58	0.55	0.53
CNG HEV	0.53	0.44	0.39	0.37	0.37
CNG PHEV	0.36	0.33	0.30	0.28	0.28
H2 FCV	0.34	0.32	0.28	0.26	0.24
H2 Hybrid FCV	0.34	0.32	0.28	0.26	0.24
H2 PHEV FCV	0.25	0.24	0.21	0.20	0.19
H2 ICE	0.45	0.44	0.41	0.40	0.38
BEV	0.20	0.19	0.16	0.15	0.15

Table D.14: PPV Fuel Consumption $[kWh/km]^{60}$

	2015	2020	2030	2040	2050
Diesel	1.01	0.86	0.77	0.75	0.71
Diesel HEV	0.81	0.69	0.61	0.60	0.57
Diesel PHEV	0.54	0.49	0.42	0.40	0.38
CNG	1.25	1.22	1.17	1.08	1.03
CNG HEV	1.00	0.98	0.94	0.86	0.82
CNG PHEV	0.62	0.60	0.56	0.51	0.49
\mathbf{LNG}	1.25	1.22	1.17	1.08	1.03
LNG HEV	1.00	0.98	0.94	0.86	0.82
\mathbf{BEV}	0.31	0.30	0.25	0.23	0.22
H2 FCV	0.61	0.52	0.46	0.45	0.43
LH2 FCV	0.61	0.52	0.46	0.45	0.43

Table D.15: LDV Fuel Consumption $\left[kWh/km \right]^{61}$

⁶⁰Own calculations based on EWI et al. (2014), Dodds and McDowall (2014), Dodds and Ekins (2014), DLR et al. (2012), dena and LBST (2017), PLANCO Consulting (2007) and Papadimitriou et al. (2013). ⁶¹Own calculations based on EWI et al. (2014), Dodds and McDowall (2014), Dodds and Ekins (2014), DLR et al. (2012), dena and LBST (2017), PLANCO Consulting (2007) and Papadimitriou et al. (2013).

	2015	2020	2030	2040	2050
Diesel	2.45	2.30	2.10	1.90	1.77
Diesel HEV	1.72	1.61	1.47	1.33	1.24
CNG	2.54	2.36	1.97	1.88	1.79
CNG HEV	1.78	1.65	1.38	1.31	1.25
\mathbf{LNG}	2.54	2.36	1.97	1.88	1.79
LNG HEV	1.78	1.65	1.38	1.31	1.25
\mathbf{BEV}	0.80	0.80	0.80	0.80	0.80
H2 FCV	1.47	1.38	1.26	1.14	1.06
LH2 FCV	1.47	1.38	1.26	1.14	1.06

Table D.16: HDV Fuel Consumption $\left[\rm kWh/\rm km\right]^{62}$

 $[\]overline{^{62}}$ Own calculations based on EWI et al. (2014), Dodds and McDowall (2014), Dodds and Ekins (2014), DLR et al. (2012), dena and LBST (2017), PLANCO Consulting (2007) and Papadimitriou et al. (2013).

	Fuel Type	2015	2050	Sources
	Gasoline/Diesel	10	10	
	Gas	65	30	
	Liquefied Gas	40	20	Krewitt and Schmid (2005),
Investment Cost [EUR/kw]	H2	350	100	Mariani (2016), Schmidt et al. (2016)
	LH2	280	100	
	Electricity	550	350	
Interest Rate [%]	All	10	10	Platts (2016)
Lifetime [a]	All	25	25	IEA (2013)
	Gasoline/Diesel	3.2	3.2	
FOM Cost [% of investment cost]	Gas	0.4	0.4	
	Liquefied Gas	3.2	3.2	
	H2	2.9	2.9	Schmidt et al. (2016)
	LH2	2.9	2.9	
	Electricity	1.0	1.0	
	Gasoline/Diesel	0.05	0.05	
	Gas	11	7	
Variable Crat [FUD /MWh]	Liquefied Gas	5	5	
variable Cost [EUK/MWn]	H2	15	15	EA (2013)
	LH2	5	5	
	Electricity	0.1	0.1	
Full Load Hours	All	2000	2000	IEA (2013)
	Gasoline/Diesel	1.0	1.0	
	Gas	1.0	1.0	
Fuel Distribution Costs to	Liquefied Gas	2.3	2.3	Balat (2008), Dodds and
[EUR/MWh]	H2	13.2	13.2	McDowall (2014), IEA (2013), Yang and Ogden (2007)
. , ,	LH2	3.0	3.0	
	Electricity	6.7	6.7	

Table D.17: Techno-economic assumptions for refueling/charging stations as well as fuel distribution costs to refueling/charging stations as used in the road transport module $\frac{1}{2}$

Appendix E. Additional information regarding application of integrated model

Appendix E.1. Supporting information scenario framework

The CO₂ constraint in the electricity market module covers cumulative emissions from electricity generation across all European countries, regardless of the sector that uses the electricity. In the scenario at hand, the aim is to reduce not only the direct emissions from, e.g., the burning of fossil fuels but the upstream emissions as well. Within the electricity market module, upstream emissions may result from, e.g., coal mining or biofuel production. Historical data on European greenhouse gas emissions is taken from the European Environmental Agency (EEA (2017)).⁶³ For 2020, an emission reduction of 24% compared to 2005 emission levels is set for the European electricity sector.⁶⁴ Furthermore, the scenario requires that emissions decline by 43% compared to 2005 emission levels by 2030 and 90% compared to 1990 by 2050. All percent values are based on official reduction targets formulated by European Commission (2014).

For the road transport sector, the CO_2 constraint is implemented as a percentage reduction of CO_2 equivalent emissions emitted not for Europe as a whole, but rather for each individual European country. Whereas policies to decarbonize the electricity sector tend to be regulated on the European level (e.g., via instruments such as the EU-ETS), the road transport sector is assumed in this scenario to be overseen nationally. The decarbonization target for the road transport sector applies to both the TTW and the WTT emissions. Historical emissions data is based on the EEA (2017) and UBA (2017).⁶⁵ National reduction targets for the road transport sector are based on the Effort Sharing Decision of the European Commission for 2020 European Commission (2009) and 2030 European Commission (2016b) for each European member state and can be found in Table E.18. For 2050, CO_2 emissions in the transportation sector are to be reduced by 90% compared to 1990 values in every country, consistent with the electricity sector target. The energy transformation module is not subject to a CO_2 reduction target. The produced zero-carbon and carbon-neutral ptx fuels, however, contribute to the targets imposed on the electricity and road transport sectors, depending on the sector in which the fuels are consumed.

⁶³Historical values were adjusted to account for upstream emissions.

 $^{^{64}}$ The European 2020 Climate & Energy Package outlines a 21% reduction relative to 2005 emission levels European Commission (2014). However, latest developments and discussions have shown that this target is likely to be surpassed and was therefore adjusted accordingly in the model.

 $^{^{65}\}mathrm{Historical}$ values were adjusted to account for the WTT emissions.

	2020			2030			
	$MtCO_2$	Target (cp. 20	15)	$MtCO_2$	Target ((cp. 2005)	
AT	19.1		-5%	13.9		-36%	
\mathbf{BE}	25.4	-	10%	18.0		-35%	
\mathbf{BG}	9.0		4%	7.4		0%	
\mathbf{HR}	6.5		4%	5.5		-7%	
\mathbf{CZ}	17.6		5%	13.8		-14%	
DK (East)	5.1	-	13%	3.8		-39%	
DK (West)	6.0	-	13%	4.4		-39%	
\mathbf{EE}	2.2		2%	1.7		-13%	
\mathbf{FI}	12.1		-8%	9.0		-39%	
\mathbf{FR}	143.8		-7%	100.8		-37%	
\mathbf{DE}	170.4		-7%	113.2		-38%	
\mathbf{GB}	126.0		-6%	89.5		-37%	
\mathbf{GR}	20.4		2%	20.4		-16%	
\mathbf{HU}	12.1		10%	9.9		-7%	
\mathbf{IE}	10.9	-	13%	9.4		-30%	
\mathbf{IT}	108.0		-3%	86.8		-33%	
\mathbf{LV}	2.8		5%	2.5		-6%	
\mathbf{LT}	2.6		44%	3.5		-9%	
\mathbf{NL}	29.9	-1	10%	23.4		-36%	
NO	10.7		-7%	6.8		-38%	
\mathbf{PL}	48.4		3%	34.7		-7%	
\mathbf{PT}	19.7		3%	18.4		-17%	
RO	14.5		10%	10.7		-2%	
\mathbf{SK}	6.1		6%	5.5		-12%	
\mathbf{SI}	5.1		1%	3.6		-15%	
\mathbf{ES}	82.2		-4%	75.0		-26%	
\mathbf{SE}	19.7		-8%	14.4		-40%	
\mathbf{CH}	15.6		-7%	10.7		-38%	

Table E.18: Decarbonization targets for the road transport sector, based on the EU Effort Sharing CO₂ Targets



Figure E.2: Assumptions on fossil fuel and CO_2 feedstock (from direct air capture) price developments based on IEA (2016b), DLR et al. (2014), Krewitt and Schmid (2005), EIA (2015), Henderson (2016) and Schmidt et al. (2016). Fossil fuel prices include any production costs (e.g., oil refining or methane reformation) and exclude taxes and fees.

Appendix F. Supplementary results of the integrated multi-sectoral model (coupled)

Appendix F.1. Additional European road transport results

The marginal CO_2 abatement costs for single countries are shown in Table F.19.

	2015	2020	2030	2040	2050
AT	0	147	0	114	496
\mathbf{BE}	0	175	112	121	497
\mathbf{BG}	0	0	0	0	496
\mathbf{HR}	0	0	0	42	496
\mathbf{CZ}	0	0	0	130	501
DK (East)	0	175	100	116	496
DK (West)	0	175	96	116	496
\mathbf{EE}	0	0	0	0	469
\mathbf{FI}	0	175	0	0	470
\mathbf{FR}	0	175	73	59	496
\mathbf{DE}	0	168	70	92	499
\mathbf{GB}	0	168	80	88	496
\mathbf{GR}	0	0	0	0	496
\mathbf{HU}	0	0	0	35	496
IE	0	175	0	63	499
\mathbf{IT}	0	0	0	0	496
\mathbf{LV}	0	0	0	0	495
\mathbf{LT}	0	903	0	0	481
NL	0	175	0	46	496
NO	0	114	25	6	496
	0	129	110	137	501
PT	0	0	0	0	496
RO	0	0	0	111	496
SK	0	0	0	57	497
SI	0	0	40	130	498
ES	0	168	0	124	501
SE	0	175	0	0	488
\mathbf{CH}	0	175	75	105	496

Table F.19: Marginal CO₂ Abatement Costs, Road Transport Sector [EUR/tCO2]

Appendix F.2. Developments in the European electricity sector

One of the main objectives of the research at hand is to develop a consistent, integrated multi-sectoral energy system model that can be used to understand the cross-sectional effects under the increased electrification of fuel production and road transport. The scenario results for the European road transport sector shown in Section 3.2 reveal that both electric vehicles and ptx fuels will play an important role in reaching the sector-specific decarbonization targets. Because of the endogenous nature of the model presented, the consequences of these changes in fuel consumption patterns in the electricity sector can be quantified.

Figure F.3 shows the results of the electricity capacities and generation in Europe in 2020, 2030 and 2050. The overall installed capacity in Europe more than doubles, from 1160 GW in 2020 to 2660 GW in 2050. Declining costs as well as the sector-specific European CO_2 target drives the investments in renewable energy, which ultimately dominate the electricity mix. For the European conventional power plant fleet, decarbonization drives a switch from coal- to gas-fired power plants. In 2050 there is a large share of open-cycle gas turbines (OCGT) which serve as backup capacities, offering security of supply under high penetration of VRE. The net electricity generation in Europe rises from 3600 TWh in 2020 to 4950 TWh in 2050. Renewable energy resources comprise 54 % in 2030 and 88 % in 2050 of all European electricity produced. Wind power yields the largest share with 40 % in 2050, followed by PV with a share of 30 % of total electricity generation in 2050.



Figure F.3: Installed electricity capacity (left) and generation (right) in Europe in 2020, 2030 and 2050 in the coupled model

The developments in the European road transport sector described in Section 3.2 drive a significant increase in electricity demand over time. As such, the investments in electricity capacities between 2030 and 2050 shown in Figure F.3 are made, in part, to generate electricity to serve the additional electricity demand from road transport and ptx processes. As shown in Figure F.4, the exogenous demand before ptx and electric mobility decreases over time due to, among others, efficiency improvements. Nevertheless, electrolysis, integrated Fischer-Tropsch and liquefaction systems, accounting for nearly 130 GW_{el} in 2050, demand an additional 630 TWh of electricity to serve fuel-cell and natural gas PPVs, LDVs and HDVs. An additional 570 TWh of electricity is consumed directly by BEVs. As a result, the European electricity demand is increased by nearly 33 % in 2050, from 3675 TWh to 4870 TWh.



Figure F.4: Electricity consumed by the exogenous electricity demand as well as the endogenous ptx and road transport demand in Europe in 2020, 2030 and 2050 in the coupled model (left); Results of the marginal electricity generation costs (weighted-average across all EU countries) and marginal CO_2 abatement costs for the electricity sector in the coupled model (right)

The average short-term marginal costs of electricity generation across all European countries are shown in Figure F.4. The average European marginal costs of electricity generation increases from 38 EUR/MWh in 2030 to 58 EUR/MWh by 2050. Increasing investments in VRE, which are needed to achieve the sectorspecific decarbonization target, require investments in flexible backup capacities to ensure security of supply. Also, changes in variable costs of price-setting power plants due increasing fuel price projections or fuel switches may increase average marginal electricity generation costs. Countries with lower marginal costs tend to build VRE capacity for export into other EU countries. In 2050, large NTC capacities allow the electricity prices across Europe to converge, as electricity imports and exports are often unrestricted until equilibrium is reached. Finland, for example, exhibits the lowest marginal costs of electricity generation at 50 EUR/MWh and Italy the highest at 67 EUR/MWh in 2050 (Table F.20).

The marginal CO₂ abatement costs in the European electricity sector, driven by the sector-specific European-wide decarbonization target of -90 % compared to 1990, are also shown in Figure F.4. Between 2020 and 2030, Europe relies on low-cost decarbonization options such as a gradual switch from coal to gas and renewable expansion at cost-efficient locations. In particular, because the model is designed as a social planner problem with perfect foresight, it anticipates the 2050 emissions target. Restrictions on yearly capacity additions increase investments in low-emission generation capacities ahead of time, causing a gradual decrease in the marginal CO₂ abatement costs. By 2030, the marginal CO₂ abatement costs sink to 2 EUR/tCO_2 , as investments in VRE have relaxed the CO₂ constraint. After 2030, the decarbonization target becomes more restrictive, pushing the CO₂ price to reach just over 75 EUR/tCO₂ by 2050. Because

of the consistent, integrated nature of the model, the marginal costs of electricity generation as well as the marginal CO_2 abatement costs of the electricity sector properly account for the endogenous demand from electric vehicles and ptx systems. As such, the electricity sector enables not only the decarbonization of itself but also of major parts of the road transport sector, both via the increased electrification and ptx fuel production.



Appendix F.3. Developments in energy transformation technologies

Figure F.5: Installed capacities (left) as well as electricity consumption and fuel production (right) of ptx and liquefaction technologies in Europe between 2030 and 2050

Appendix G. Supplementary assumptions and results of the decoupled model



Appendix G.1. Exogenous parameters

Figure G.6: Exogenous ptx fuel and electricity prices assumed in the decoupled model

Appendix G.2. Selected delta comparisons

	2015	2020	2030	2040	2050
AT	0	17	0	-40	27
\mathbf{BE}	0	-6	0	65	27
BG	0	0	0	0	27
\mathbf{HR}	0	0	0	-42	27
\mathbf{CZ}	0	0	0	-8	23
DK (East)	0	-6	7	-27	27
DK (West)	0	-6	12	-26	27
\mathbf{EE}	0	0	0	0	55
FI	0	-6	11	70	54
\mathbf{FR}	0	-6	19	10	27
\mathbf{DE}	0	-4	36	-22	25
\mathbf{GB}	0	2	13	-10	27
\mathbf{GR}	0	0	0	0	27
\mathbf{HU}	0	0	0	-35	27
\mathbf{IE}	0	-6	0	11	25
\mathbf{IT}	0	0	0	0	27
\mathbf{LV}	0	0	0	0	29
\mathbf{LT}	0	5	0	0	42
\mathbf{NL}	0	-6	0	24	27
NO	0	56	83	84	27
\mathbf{PL}	0	12	2	49	32
\mathbf{PT}	0	0	0	0	27
RO	0	0	0	10	27
\mathbf{SK}	0	0	0	-41	27
SI	0	0	13	-9	25
\mathbf{ES}	0	-4	0	19	27
\mathbf{SE}	0	-6	11	70	36
CH	0	-6	18	-15	27

Table G.21: Delta Marginal CO_2 Abatement Costs, Road Transport Sector (decoupled minus coupled) [EUR/tCO2]

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