Electricity Tariff Engineering for Integrated Energy Systems

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CHAPTER 1

LIST OF ABBREVIATIONS

ANFIS	Adaptive Neuro-Fuzzy Inference System
ANN	Artificial Neural Network
ARIMA	Seasonal Auto-Regressive Integrated Moving Average
ARMA	Auto-Regressive Moving Average
CNN	Convolutional Neural Network
CPP	Critical Peak Pricing
CR	Concentration Ratio
CV	Coefficient of Variation
DC	Direct Current
DET	Distributed Energy Technologies
DL	Deep Learning
DSO	Distribution System Operator
DT	Decision Tree
ELM	Extreme Learning Machine
EPEX	European Power Exchange
EV	Electric Vehicle
GARCH	Generalized Auto-Regressive Conditional Heteroskedasticity
GRU	Gated Recurrent Unit
HH	Household
HHI	Herfindahl-Hirschman Index
kV	kilovolt
kWh	kilowatthour
LFC	Load Frequency Control
LSTM	Long-Short Term Memory

MAE	Mean Absolute Error
MAPE	Mean Absolute Percentage Error
MASE	Mean Absolute Scaled Error
MLP	Multilayer Perceptron
MSE	Mean Squared Error
Mt	Megaton
PV	Photovoltaics
RMSE	Root Mean Square Error
RNN	Recurrent Neural Network
RTP	Real-time Price
SVM	Support Vector Machine
SVR	Support Vector Regression
TOU	Time of Use
TSO	Transmission System Operator

Part I.

Fundamentals

CHAPTER 2

INTRODUCTION

One of the greatest challenges for humanity in the 21st century is the mitigation of the climate crisis. Mitigating climate change requires a strong reduction of greenhouse gases (IPCC, 2021) and thus the replacement of various existing fossil-fuel based technologies and processes. In many cases, the most viable and economic substitutes are technologies and processes, which run on CO_2 free electricity. These novel technologies, like heat pumps, electric vehicles, and electrolyzers, use large amounts of electricity, and are, therefore, strongly linked with the electricity system. Given the already complex nature of the electricity system, and the additional challenges introduced by volatile renewable electricity generation, it is of utmost importance to integrate these novel technologies in a way that minimizes societal costs. To achieve this, current electricity tariffs – the prevalent mechanisms that economically connect electricity users and technologies to the rest of the system – need to be analyzed and updated for the era of integrated energy systems. Electricity tariffs can be seen as "[...] the nervous system of the power sector, helping coordinate the diverse interests of the dispersed actors engaging with the world's most complex machine — the power grid." (Burger, 2019, p. 21). More concretely, tariffs are sets of rules that define how customers are charged for their electricity consumption. The theoretical tenets of economically efficient tariff design are well-known, yet tariffs applied in practice mostly remain inefficient. Inefficient tariffs have been shown to strongly increase societal costs of the electricity system (Borenstein, 2005; Faruqui et al., 2010; Itron, 2017), even in the ending fossil-fuel era. These effects will be greatly amplified and complicated with the disruptive uptake and integration of new technologies: "The growing integration [of energy technologies] increases the importance of well-designed economic signals and the ramifications of poorly designed signals" (Pérez-Arriaga and Knittle, 2016, p. 75). Therefore, well-engineered tariffs are crucial for a successful integration of new technologies in the energy system, and for a successful mitigation of the climate crisis.

2.1 Motivation

Currently, around three-quarters of greenhouse gas (GHG) emissions are caused by the burning of fossil fuels (International Energy Agency, 2021a). The by far most important sectors that cause fossil fuel combustion are buildings, transport, and industry. Their combined emissions have still risen in recent decades and amount to almost 30 Gigatonnes CO_2 as of 2019 (Figure 2.1). To get these sectors to zero emissions, existing fossil-fuel based technologies and processes must be replaced by novel ones that allow the usage of CO_2 free electricity.

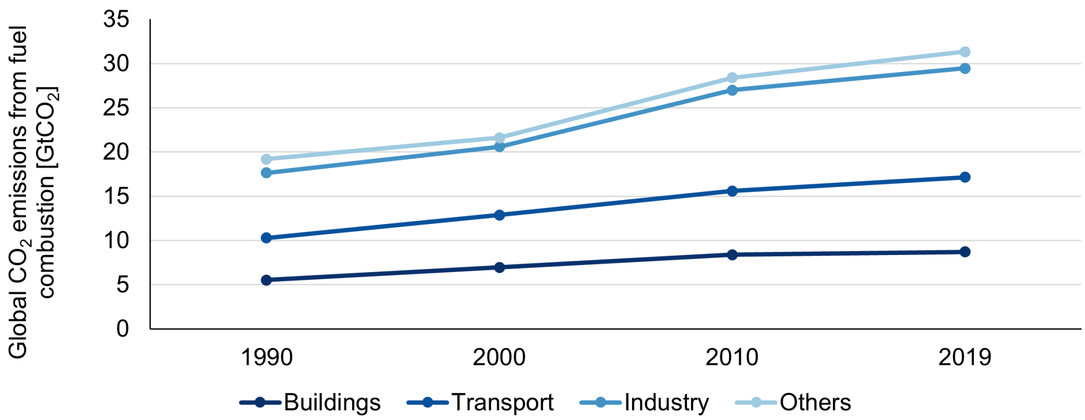


Figure 2.1.: Development of global CO_2 emissions from fuel combustion by sector (stacked) (International Energy Agency, 2021a)

In the building sector, the greatest electrification opportunity consists of converting gas and oil heaters to electric heat pumps (International Energy Agency, 2021c). For the electricity production for heat pumps, roof-top solar photovoltaic (PV) plants, oftentimes combined with home battery storage systems, will play a large role. Solar PV, batteries, and heat pumps have already seen a rapid uptake in recent years. Figure 2.2 displays the installations for the building sector in Germany. After strong growth in recent years, there are about one million solar PV plants, 300,000 residential batteries, and 1.1 million heat pumps in Germany as of

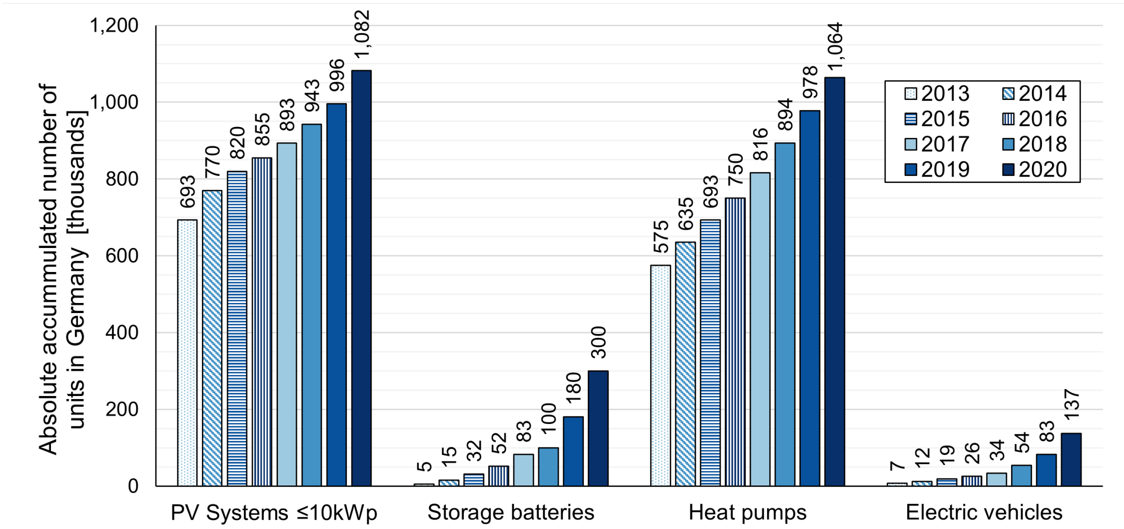


Figure 2.2.: Diffusion of various energy technologies in Germany. Own representation, based on Schulz and Hufendiek (2021). Data from Bundesnetzagentur (2021), Institut für Stromrichtertechnik und Elektrische Antriebe (2019), Bundesverband Energiespeicher (2021), Bundesverband Wärmepumpe (2021), and Kraftfahrt-Bundesamt (2021).

2020. The growth of adoption will further accelerate, if net zero GHG emissions are to be reached. For example, if Germany wants to be climate neutral by 2045, it is estimated that 5.5 million heat pumps need to be installed by 2030 (Kemmler et al., 2021). Globally, *annual* sales of around 60 million heat pumps are needed in order to achieve net zero by 2050 (International Energy Agency, 2021c).

In the transport sector, emissions are mainly caused by passenger road vehicles and road freight vehicles (International Energy Agency, 2019b). For substituting those, battery electric vehicles (BEVs) and, for long distance transportation, fuel cell electric vehicles (FCEVs) powered by electrolytic hydrogen are the key technologies that enable electrification and thus zero emissions (Ueckerdt et al., 2021; International Energy Agency, 2021c). The diffusion of BEVs has accelerated in recent years, as Figure 2.2 shows. Currently, there are around 137,000 BEVs on German roads. Similar to solar PV plants, batteries, and heat pumps, BEVs are set to see further strong growth: 16 million electric cars will be needed in Germany by 2030 on the path to climate neutrality in 2045 (Kemmler et al., 2021). Worldwide, an estimated 1.6 billion electric cars are needed by 2050 to reach net zero climate emissions (International Energy Agency, 2021c).

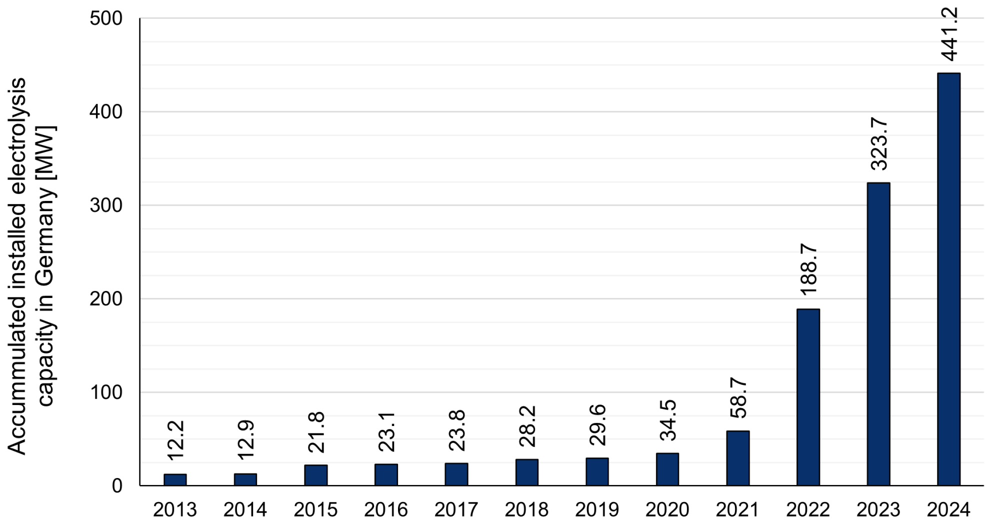


Figure 2.3.: Diffusion (historical and scheduled) of electrolysis capacity in Germany. Based on Heymann et al. (2021) and own research (see Table A.1 in the Appendix).

In the energy intensive industry, some processes are difficult or impossible to electrify directly. Here, the use of hydrogen produced by electrolysis with GHG-free electricity is a key technology to reach climate neutrality (Ueckerdt et al., 2021; International Energy Agency, 2021c). Installed electrolysis capacity is experiencing strong growth, reaching an estimated total of 58.7 MW in 2021 in Germany (Figure 2.3). This growth is set to accelerate, with forecasted capacities of 6,500 - 9,500 MW in Germany by 2030 (Kemmler et al., 2021; SPD, BÜNDNIS 90 / DIE GRÜNEN and FDP, 2021; vom Scheidt et al., 2022).

Since heat pumps, electric vehicles, and electrolyzers have high electricity demands, they inevitably strongly interact with the electricity system. Depending on how they are adopted and operated, new technologies can either decrease or increase grid congestion (Staudt et al., 2018a; vom Scheidt et al., 2022; Salah et al., 2015), emissions (Huber et al., 2021; Itron, 2017; vom Scheidt et al., 2022), and usage of renewable electricity (Schuller et al., 2015).

This creates the challenge to analyze current economic mechanisms that impact the integration of new electricity consumption, generation and storage technologies, and to update them adequately. The prevalent mechanism for this task is the electricity tariff. Given the important role of tariffs, there is already a large body of related research on tariff effects in conventional electricity systems without innovative, energy-intensive technologies. Well-designed tariffs are known to incentivize both efficient utilization of existing generation and transmission infrastructure as well as to send efficient investment signals for new infrastructure (Borenstein, 2005). On the other hand, ill-designed tariffs can incentivize inefficient adoption of roof-top solar PV (Simshauser, 2016), increase costs for society (Imelda et al., 2018) and increase emissions (Itron, 2017), thus significantly hindering the energy transition. In terms of economic savings, Borenstein (2005) estimates that improving tariff design could save 5% - 10% of electricity costs in California in the long run, and Faruqui et al. (2010) estimate that moving to dynamic tariffs in the European Union (EU) could save around 50 billion Euro annually.

The substantial effects of tariff design, either positive or negative, can be expected to multiply with the advent of new, electricity based technologies (Pérez-Arriaga and Knittle, 2016). Consequently, policy makers as well as energy companies have called for more consumer-centric electricity markets (European Commission, 2017a,b; Elia Group, 2021). The European *Agency for the Cooperation of Energy Regulators* has explicitly asked the national regulatory authorities to "enable consumers to receive appropriate price signals" that incentivize system-beneficial integration of new technologies in the electricity system (European Union Agency for the Cooperation of Energy Regulators, 2021).

With this thesis, I contribute to our knowledge of the interplay of tariff engineering and technology integration through multiple rigorous quantitative analyses, and I derive concrete implications and recommendations for residential consumers, energy retailers, customer advocates, regulators, and politicians. The thesis has a global scope, with case studies for Germany, the UK, and the USA, and is logically structured into two parts.

The first part addresses the integration of small-scale energy technologies at the local level, i.e. the interplay of tariffs and residential heat pumps, electric vehicles, roof-top solar PV panels, and residential batteries. In the status quo, these technologies are commonly facing time-invariant "flat" volumetric household tariffs. Such flat tariffs set inefficient economic signals that obscure the underlying value of electricity, whereas tariffs with time-variant pricing can increase efficiency and societal welfare

(Joskow, 2007; Borenstein and Holland, 2003; Desai and Dutta, 2013). Despite their clear economic benefits for the system, new tariff designs are not popular among residential customers and electricity retailers in Europe. Only in 11 of 27 states in the EU, electricity consumers even have the option to choose a real-time or hourly tariff (European Union Agency for the Cooperation of Energy Regulators, 2021). In Germany, less than 0.1% of standard load profile customers (which include all regular residential customers) have the electricity metering infrastructure required to use dynamic tariffs (Bundesnetzagentur and Bundeskartellamt, 2021). To facilitate the uptake of time-varying tariffs, I engineer and evaluate decision support tools and forecasts that support customers to select and use individually optimal electricity tariffs, and even bundles of tariffs, smart meters, and energy technologies. The results uncover substantial synergies of time-varying tariffs and flexible new energy technologies, which unlock much higher cost reductions for customers than tariff-switching alone. Besides, with innovative Machine Learning algorithms that make use of short smart meter data fragments, reliable individual tariff-technology bundle recommendations can be given to customers one year in advance. To enable the optimal operation of these technologies once they are installed, I review, design, and evaluate forecasts that deliver valuable information about short-term future net electricity loads and serve as crucial inputs for the a priori scheduling of technologies under different tariffs. In combination, these forecasts and decision support tools can facilitate the uptake of new technologies and efficient tariffs amongst residential customers.

Zooming out from the local, residential customer level, the second part of this thesis addresses the integration of large-scale electrolyzers at the system level and the effects of electricity tariffs, thereon. On the system level, both the temporal and the spatial dimension of tariff signals can play a large role. Hence, I engineer tariffs with different temporal and spatial resolutions and assess their effects on the optimal hydrogen supply chains, end-use hydrogen costs, and the integration of hydrogen in the electricity system, in the form of grid congestion management costs, and CO_2 emissions. The results show that the integration of electrolyzers in the German system under current uniform price regulation causes a large increase in congestion management costs of over one billion Euro per year, and a large increase in emissions of about two Megatons (Mt) CO_2 per year. This is contrasted with a case of efficient spatial economic tariff signals, which incentivize much more system-friendly integration, causing a decrease in congestion management costs of over one billion Euro per year (i.e. a delta of over two billion Euro annually), and a decrease in emissions of over three Mt CO_2 (i.e. a delta of over five Mt annually). The largest cost reduction can be achieved when the tariff contains both spatial and temporal information. These new findings deliver important information to policy makers in single-price electricity markets, such as Germany, as they demonstrate the considerable benefits of spatially differentiating the economic signals for the thousands of Megawatts of electrolyzer capacity that are to be built in this decade.

In summary, this dissertation proposes, evaluates and discusses efficient tariff designs and related tools for well-integrated energy systems at the distribution and the transmission grid level. It thus provides guidance for energy retailers, customer advocates, regulators, and policy makers to make well-informed decisions that increase societal welfare. This way, I aim to contribute to a successful transition to more sustainable energy systems and global climate neutrality.

2.2 Research Questions

The high potential benefits of dynamic tariffs, and their extremely low adoption rates amongst residential customers motivate the search for a reliable tariff recommendation tool that can foster the uptake of innovative, system-beneficial tariffs by individual consumers in the easiest way. Therefore, Research Question 1 refers to the recommendation of tariffs to end-consumers with a naive approach. Research Question 2 covers the consequences for customers' electricity bills of such recommendations.

Research Question 1 *What is the performance of a naive tariff recommendation approach based on historical data?*

Research Question 2 *What are the economic consequences of these recommendations for customers?*

The answers to these research questions regarding statistical performance and economic saving potentials uncover the need for recommendation methods that are more sophisticated and combine the recommendation of tariffs and technologies. Therefore, Research Question 3 addresses the performance of Machine Learning methods for recommending such bundles. Research Question 4 again addresses the financial consequences for customers that follow the developed recommendations.

Research Question 3 *What is the performance of Machine Learning based methods for recommending bundles of tariffs and technologies to end-consumers?*

Research Question 4 *What are the economic consequences of these recommendations for customers?*

Tariffs and technologies find the highest synergies when tariffs set the right price signals while technologies are operated in a cost-optimized fashion. To plan such operation in advance, proper forecasting of future household electricity demand is very important. Therefore, the status quo of electric load forecasting is reviewed. The findings answer Research Question 5. Based on the insights from this review, a forecasting model is developed and applied to a relevant case study, concerning the performance of load forecasts at household level. To answer Research Question 6, it is then analyzed how the quality of such forecasts differs for households with novel energy technologies.

Research Question 5 *What are state of the art methodological approaches for electric load forecasting in the literature?*

Research Question 6 *What is the performance of Machine Learning sequence models for forecasting residential electric loads in the presence of roof-top solar and electric heating installations?*

The above questions target small-scale technologies at the local level. On a larger scale, and more concentrated, electrolysis technology will be installed. Hydrogen, produced via electrolysis, can be expected to introduce new large loads to the electricity transmission grid. Uniquely, hydrogen can be used as a transportable energy carrier itself. This raises the question whether it should be produced at the locations of end-use (i.e. next to hydrogen consumers), or at the locations where cheap electricity is available. To showcase and quantify this trade-off, a comprehensive model of the German electricity and hydrogen system in 2030 is developed, and evaluated. First, the supply chain's volume and its optimal technologies are identified in response to Research Question 7. To analyze the effect of tariffs in this context, Research Question 8 is posed. Since hydrogen will also have considerable feedback effects on the electricity system, Research Question 9 analyzes how the hydrogen supply chains that emerge under different tariffs impact wholesale electricity prices, congestion management costs, and emissions.

Research Question 7 *What is the cost-minimal supply chain design using electrolytic hydrogen production for the combined hydrogen demand from all major relevant sectors in 2030 in Germany?*

Research Question 8 *What is the effect of electricity tariffs on cost-minimal locations of electrolyzers and hydrogen costs?*

Research Question 9 *How does hydrogen production change electricity wholesale prices, congestion management costs, and CO_2 emissions under different tariffs?*

The thesis puts a particular focus on data-driven analyses and employs methods from mathematical optimization and Machine Learning. Thus, it delivers quantitative answers to most posed research questions.

2.3 Thesis Structure

This thesis is structured as depicted in Figure 2.4. First, after this introduction (Chapter 2), the fundamentals of electricity markets and tariffs are presented, to provide the necessary background knowledge for the subsequent chapters. Chapter 3 has two sections. In the first, the principles of wholesale electricity markets are introduced. In the second, the fundamentals of electricity retail markets and the status quo of the German retail market are described. In Chapter 4, the fundamentals of electricity tariffs are outlined. This constitutes Part I.

Then, the two main parts of the thesis follow, structured according to the two different analyzed levels of the power system. For the end customer level, Part II covers the design of time-varying electricity tariffs and recommendation solutions for the integration of roof-top solar PV plants, home batteries, electric cars, and

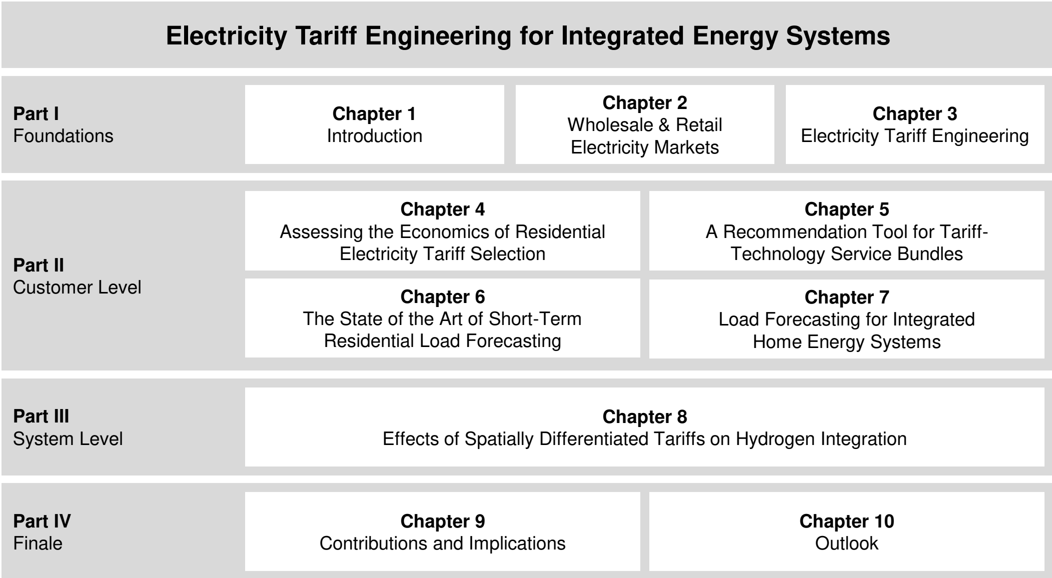


Figure 2.4.: The structure of this thesis

residential heat pumps (Chapter 5 and 6). Besides, state-of-the-art data analytics methods for forecasting of residential loads are reviewed (Chapter 7) and a novel forecasting method is presented for residential loads that are influenced by solar PV plants and heat pumps (Chapter 8).

For larger-scale technology at the system level, Part III puts the focus on the role of spatially differentiated electricity tariffs for the integration of large-scale hydrogen infrastructure (Chapter 9).

Finally, in Part IV, the answers to the research questions are summarized and the key contributions of this thesis are distilled (Chapter 10). Furthermore, an outlook for further research is provided (Chapter 11).

Chapters 5 to 9 rely on or comprise published articles, or working papers. In all cases, I disclaim this clearly at the beginning of the respective chapters. Within those chapters, I consistently refer to the authors as “we”, since I collaborated with fellow researchers for these articles.

CHAPTER 3

ELECTRICITY MARKETS

Electricity is an important good that affects many essential areas of society and economy (Petermann et al., 2010). Electricity systems can be represented by two layers: a technical layer and an economic layer.

The stylized technical value chain in the electricity system can be structured into the following four steps. First, there is the *generation* of electricity. The electricity is then transported in *transmission* grids and *distribution* grids to the point of *consumption*.

Electricity generation implies the transformation of non-electric energy – such as solar radiation, kinetic energy, chemical energy, and thermal energy – into electrical energy. In order to mitigate climate change, the generation technology portfolio needs to switch from fossil fuel based sources like lignite, hard coal, and natural gas, to emission free technologies like solar PV, wind, and hydro power. In the German system, fossil fuel based electricity generation accounted for 40.9% in 2021, renewable electricity generation accounted for 45.8%, and nuclear electricity generation accounted for 13.3% (Fraunhofer, 2022).

Transmission and distribution refers to the delivery of electricity in lines. In Germany, the transmission grid is operated at voltage levels of 380 kilovolt (kV), and 220 kV, whereas the distribution grid is operated at 110 kV or lower. The German transmission grid is split up into four zones, operated by four different Transmission System Operators (TSOs). They are responsible for the stable and secure operation of their grids, which includes performing redispatch measures, when needed (Bundesnetzagentur and Bundeskartellamt, 2021). The distribution grid has a much higher number of actors, with 878 Distribution System Operators (DSOs) as of 2021 (Bundesnetzagentur and Bundeskartellamt, 2021). TSOs and DSOs typically have natural monopolies in their grid area and are therefore regulated by the German federal network agency "Bundesnetzagentur" (Bundesnetzagentur and Bundeskartellamt, 2015), the equivalent to the Federal Energy Regulatory Commission (FERC) in the USA.

Most of the final consumers (>99.99%) are connected to the distribution grid: about 49,137,900 residential customers and 2,856,400 industrial and commercial customers. Approximately 500 larger industrial customers are directly connected to the transmissions grid. In terms of electricity consumption, large consumers with over 2 GWh consumption per year make up 47% of the totally consumed 460.2 TWh in 2021. Medium consumers with annual consumption between 10 MWh and 2 GWh make up another 26%. Small consumers with under 10 MWh consumption per year represent 27% of the total consumption (Bundesnetzagentur and Bundeskartellamt, 2021).

Besides this technical layer, there is an economic layer that addresses the respective transactions of electricity. In unbundled electricity systems, generators typically sell the electricity to large industrial consumers and intermediaries on the *wholesale market*. These intermediaries then resell the electricity to small industrial, commercial and residential consumers on *retail markets*. Since electricity tariffs are price mechanisms for end consumers, electricity tariff engineering is mainly connected to the retail market. However, through intermediaries and feedback effects, tariffs are also connected to the wholesale markets. Therefore, to lay the foundation for the research presented in Part II and Part III, this chapter outlines the theoretical fundamentals of wholesale and retail markets, provides an analysis of the status quo of the German and European retail market, and derives consequences for electricity tariff engineering.

3.1 Electricity wholesale markets

Electricity wholesale markets are designed with the goal of ensuring supply of electricity in a way that is economically efficient – both in the short-run regarding dispatch and in the long-run regarding new investments – and reliable. Besides, there are sub-objectives such as simplicity, transparency, and fairness (Cramton, 2017).

Two archetypal electricity wholesale market designs have evolved worldwide: The integrated pool model – e.g. in Argentina, Chile, and California – and the exchange model – e.g. in Canada, Germany, and Japan (Mathiesen, 2011; Barroso et al., 2005; Maurer et al., 2018).

At the center of pool systems, there is an Independent System Operator (ISO), who has the role of both market and system operator and centrally schedules the dispatch of generation. At high computational expense, the ISO determines individual prices for each node in the power system for each point in time. These nodal prices (also called Locational Marginal Prices) explicitly take into account the local supply and demand for electricity, as well as network constraints and losses. Therefore, nodal prices correspond to the current value of a unit of electricity at the corresponding node (Schweppe et al., 1988; Weibelzahl, 2017).

In exchange based systems, grid operations and market operations are decoupled. Power generators, retailers, and large consumers can trade electricity at the wholesale market independently of the underlying technical grid constraints within the market zone. Thus, the market clears with a single price for the entire market zone, rather than with individual prices for each node. The market design does however consider grid constraints of electricity lines between the respective zone and its neighboring zones (Weibelzahl, 2017). In some countries, like Norway and Sweden, regulators have therefore divided the market area into multiple zones, to cater for structural regional imbalances (Bjørndal et al., 2013).[1]

One example for an exchange based system is Europe, where the European Power Exchange (EPEX) is one of the most important wholesale markets. At the EPEX, electricity is traded in day-ahead and intraday auctions, besides additional long-term products and bilateral intraday trading. Day-ahead and intraday auctions

[1]Note that wholesale market design includes a number of additional considerations that are outside of the scope of this thesis. These considerations include long-term generation adequacy (i.e. energy-only markets vs. capacity mechanisms), ancillary services, and forward markets (Bublitz et al., 2019; Cramton and Ockenfels, 2016; Hogan et al., 2005). These aspects can affect tariff designs, as, e.g. costs for generation capacity mechanisms and ancillary services can be recovered via respective regulated charges within consumption tariffs (Burger et al., 2020; Lobato Miguélez et al., 2008), and retailers can use forward markets to hedge risks.

are cleared through a single-price auction for each zone (Graf and Wozabal, 2013). Market zones oftentimes correspond to European countries (European Network of Transmission System Operators for Electricity, 2022). The resulting uniform price for the respective market zone is determined by the bid of the marginal generator in the respective hour (day-ahead market) or 15 minute interval (intraday market) (Zou et al., 2015). It has been shown that (large industrial) electricity consumers respond to the temporal variations in wholesale prices (Hirth et al., 2022). However, the trading process ignores technical grid constraints within the market zone. If the market outcome leads to a higher power flow on a transmission line than is allowed according to thermal limits or the regulatory n-1 criterion (Holttinen et al., 2011), "grid congestion" (Stoft, 2002) occurs, and post-trade corrective actions, such as re-dispatch by grid operators can be required to maintain grid stability. Depending on the frequency of such events and the cost structure of the system's generation portfolio, such congestion management measures can lead to high costs. For example, in the exchange based German system, the demand for electricity and the supply of electricity with low marginal costs diverge spatially (Egerer et al., 2016; Staudt and Oren, 2021). This is not reflected in wholesale price signals, leading to congestion management costs of over one billion Euro in 2020 (Bundesnetzagentur and Bundeskartellamt, 2021).

This inherent problem of exchange based systems might be further aggravated with the rise of new large electricity consumers, such as electrolyzers. As uniform prices do not send any locational signals for the installation of new electricity consuming technologies, there is the risk of electrolyzers being placed in locations where they strongly increase grid congestion. If regulators want to stick to exchange based wholesale market designs – as for example proclaimed by the European Network of Transmission System Operators for Electricity (European Network of Transmission System Operators for Electricity, 2021) – other spatial mechanisms are urgently needed, such as dedicated nodal hydrogen tariffs (see Part III).

Unlike large consumers, residential end consumers mostly do not engage directly in the wholesale market at this time (European Union Agency for the Cooperation of Energy Regulators, 2021). Instead, retailing companies work as intermediaries. They purchase electricity from generators at the wholesale market and then resell it to end consumers at the retail market.

3.2 Electricity retail markets

In this chapter, an overview of liberalized retail electricity markets for residential customers is provided, structured along the established Market Engineering framework (Weinhardt and Gimpel, 2006). Figure 3.1 depicts this framework. It consists of five main components: The socio-economic and legal environment, the transaction object, the market structure, the agent behavior, and the market outcome. The market structure itself consists of three sub-components, namely the micro structure, the (IT-)infrastructure and the business structure.

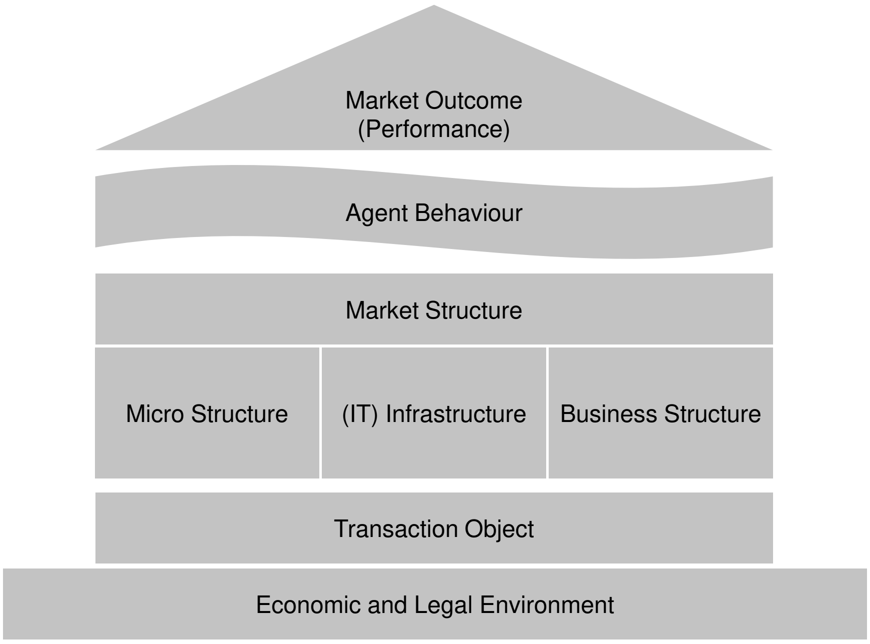


Figure 3.1.: The Market Engineering Framework by Weinhardt and Gimpel (2006)

In the following subsections, each market component is separately defined and analyzed. For this, current regulatory and academic literature is reviewed, and expert interviews with 15 stakeholders of the retail market in Germany are evaluated. These stakeholders include:

- Ten retailers, thereof four local utility retailers, two dedicated green electricity retailers, and four startups with innovative tariff models
- Two tariff comparison platforms

- One tariff switching service provider
- Two consumer rights agencies

The interviews were conducted via telephone or in written form, between June 2020 and May 2021. The interview questions are listed in Appendix B. The interview analysis does not aim to be representative of the stakeholders of the German retail market. Instead, it aims at complementing the review of literature by identifying key challenges and opportunities of innovative and conventional retailers, and revealing trends that might strongly influence the retail market in the future, but are not yet detectable in the reports published by German and European regulatory agencies.

3.2.1 Economic and legal environment

From a legal, regulatory point of view, two main types of retail electricity markets can be differentiated. Retail markets can be either liberalized or fully regulated. This section focuses on liberalized retail markets, which are the prevalent market design in Europe (European Union Agency for the Cooperation of Energy Regulators, 2021). The idea of liberalized retail markets is to allow and support competition between multiple retail companies which shall lead to low electricity costs and good services for consumers (European Union Agency for the Cooperation of Energy Regulators, 2021).[2]

Between 2016 and 2019, the EU introduced the *Clean Energy for all Europeans Package*, which comprehensively updates the market design of retail markets in the EU (European Commission, 2016; European Union Agency for the Cooperation of Energy Regulators, 2021). The package consists of eight laws, i.e. four regulations and four directives. For retail markets, the most relevant directive is *Directive (EU) 2019/944 16* (European Commission, 2019).[3]

This directive recognizes supplier switching as one of the key issues in the current retail markets in the EU and therefore proclaims that by 2026, the technical process

[2] For fundamentals of regulated retail markets and companies, see Bonbright (1961), for a current perspective see Pérez-Arriaga and Knittle (2016).

[3] Note that the directive stipulates further rules that are not discussed here, as they are not the primary focus of this thesis, e.g. referring to consumer protection and energy poverty.

of switching one's retailer must not take longer than 24 hours. This will be a considerable reduction compared to the current regulation that requires switching within three weeks (European Union Agency for the Cooperation of Energy Regulators, 2021). Therefore, this measure will reduce transaction costs for consumers and is thereby likely to increase switching rates and thus competition in the retail markets (European Commission, 2019). Faster switching procedures will require retailers to update their internal administrative processes. This can be a challenge for retailers, as one interviewed retailer calls for less bureaucracy around the switching process, and claims that they already face non-trivial transaction costs behind the scenes for switching customers (Expert 9).

Interestingly, some customer advocates and tariff comparison platform providers in Germany claim that currently, large energy retailers would try to hinder customers to switch retailers (Expert 3) and that frequently, retailers would not meet switching deadlines and delay switching processes (Expert 15). This would harm the customers and therefore, non-compliant retailers should be penalized more (Expert 15). Other stakeholders state that there are many good laws, rules, and court decisions in the German retail market that define how retailers should treat customers. However, they see that administrative authorities do not control rigorously enough, and call for higher financial penalties, for example, in the case of non-transparent price increases (Expert 10). In general, multiple stakeholders urge regulators to provide more market transparency for consumers, in order to guarantee an open, fully liberalized retail market.

Increasing information transparency for consumers is also demanded by the laws adopted as part of the Clean Energy for all Europeans Package. Amongst others, consumers' electricity bills shall contain information about actual electricity consumption, comparisons with past consumption levels and with average users, the current price and a breakdown of this price, contact information for consumer organisations, supplier information, complaint services, and switching information (European Union Agency for the Cooperation of Energy Regulators, 2021).

To further improve transparency, *Directive (EU) 2019/944 16* stipulates the need for tariff comparison tools: "Member States shall ensure that at least household customers [...], have access, free of charge, to at least one tool comparing the offers of suppliers, including offers for dynamic electricity price contracts." (European Commission, 2019). Such tools might be especially beneficial for customers who currently have a tariff contract from a primary supplier ("Grundversorger"), as default tariffs are oftentimes overpriced, as interview Expert 13 notes. However, cheaper retailers that aim for very competitive low offers might pose other risks for end consumers. European retailers that buy electricity at the wholesale market currently face extraordinarily high purchase prices (Bundesnetzagentur, 2022). These uncommonly high purchase prices have increased financial pressure on retailers that struggle to serve their end customers under long-term fixed price contracts. In Germany, 39 retailers – often smaller "discount" suppliers with particularly competitive offers – stopped operation in 2021, oftentimes referring to high wholesale prices (Groeneveld, 2022). Therefore, the current economic environment of retail markets reveals that the widespread retailer business model based on price competition, high sign-up bonuses, and low margins (as uncovered in Subsection 3.2.4) bears risk and indicates that other business models (as presented and discussed in Subsection 3.2.3) might be favorable in the future. The German Minister for Economic Affairs has recognized this and proclaims that the discounter retail business model is not resilient and that new regulation is needed to avoid such situations in the future (Matthes, 2022).

Another major trend surrounding retail markets is the increasing diffusion of smart meters. In this regard, *Directive (EU) 2019/944 16* reiterates that "Member States shall ensure the deployment in their territories of smart metering systems that assist the active participation of customers in the electricity market." (European Commission, 2019). This topic seems to be one of the major pain points for innovative retailers in Germany. Several stakeholders called for less strict regulation regarding the roll-out (Expert 1, 2, 14). They state that currently, the expenses and waiting times for certifications of software and hardware exceed the utility of the new smart meters (Expert 2). Improved regulation is hoped to facilitate the roll-out of advanced metering infrastructure, to reduce costs (Expert 2) and thus to enable innovation (Expert 14) and innovative business models (Expert 5). One expert complains that because of the high number of regulations and requirements, the first smart meter gateways could not be certified (Expert 1). With less strict regulation, more retailers might offer innovative tariff models, which would facilitate the energy transition, says one of the few retailers who offers real-time pricing (RTP) tariffs today (Expert 1). These new innovative business models are also needed to convey the usefulness of smart meters. One consumer rights agency does not see the usefulness of smart meters right now and thus is hesitant regarding a quick roll-out of more expensive smart meters for residential customers (Expert 13).

A point that is often raised in the interviews is high bureaucracy. Multiple retailers specifically call for simplifying the German law for renewable energy (Expert 4, 7, 9), as well as reducing bureaucratic effort in the retail market in general (Expert 7, 9). Besides, stakeholders call for updating the legal environment regarding regulated parts of electricity tariffs. Specifically, they ask for re-designing grid tariffs to improve the integration of distributed generation capacity, enabling the establishment of new products like the marketing of flexibility options, and integrating prosumers in a way that relieves the distribution grid (Expert 2). Moreover, they request emission certificate prices that reflect the externalities of electricity generation (Expert 6), reduction of charges and fees (Expert 8, 11), and changes to the current fixed feed-in tariffs for residential solar PV panels that enable more innovative business models for small-scale electricity generators (Expert 5).[4]

In summary, the stakeholder interviews uncover numerous regulatory hurdles for reliable and efficient retail markets. Some of those are addressed by the current EU *Clean Energy for all Europeans Package*. The announced changes to the legal framework in EU retail markets aim to simplify retailer switching, increase availability of comparison tools, and strengthen the diffusion of smart meters. In combination, these trends can be expected to facilitate the uptake of dynamic tariffs in retail markets. Attention should be given to the administrative effort of retailers, who already complain about high levels of bureaucracy that might be further increased with additional laws.

[4]Notably, one retailer requested the undoing of the unbundling of retail and generation companies (Expert 11).

3.2.2 Transaction object

The transaction object of retail markets is electricity. Electricity is physically a homogeneous good. Nevertheless, the contracts between retailer and consumer can further specify how this good is priced, where it comes from, which technical properties it has, how associated risks are allocated, and what infrastructure is required or supplied for the contract (Salah et al., 2017). These criteria are subject to the respective contract under which the good electricity is provided to the consumer and they are therefore discussed in more detail in the following Subsection 3.2.3

3.2.3 Micro structure

The microstructure defines the market mechanism, under which resources are allocated and priced (Dauer et al., 2017). In the context of retail markets, electricity tariffs are the prevalent micro structure.

Tariffs can be differentiated regarding various criteria: pricing, technical properties, risk allocation, add-on products and services, communication medium, and give-aways.[5]

Regarding pricing, tariffs can contain prices with different temporal and spatial granularity, different timing of price change announcements (a priori vs. real-time), different calculation concepts (e.g. per-kilowatthour (kWh) billing vs. fixed flat rates), and different calculation units (paying for kWh vs. paying for km travelled with an electric vehicle (EV)). The most prevalent tariff type in Europe and in many other geographies worldwide, is the Flat tariff with a time invariant per-kWh price (European Union Agency for the Cooperation of Energy Regulators, 2021; U.S. Energy Information Administration, 2021). Alternatives with time-varying prices are time-of-use (TOU) tariffs, real-time pricing (RTP) tariffs, and critical peak pricing (CPP) tariffs. These tariffs hold large potential system-benefits, as they better reflect the actual value of electricity (see Chapter 4 for details on tariff design theory). In the 28 countries of the ACER 2020 report (EU and Norway), Flat tariffs are available in all countries, whereas TOU tariffs are only available in 14, RTP in 11, and CPP in

[5]Besides tariffs offered on the free retail market, there are regulated cheaper social electricity tariffs for financially vulnerable consumers in some countries (European Union Agency for the Cooperation of Energy Regulators, 2021).

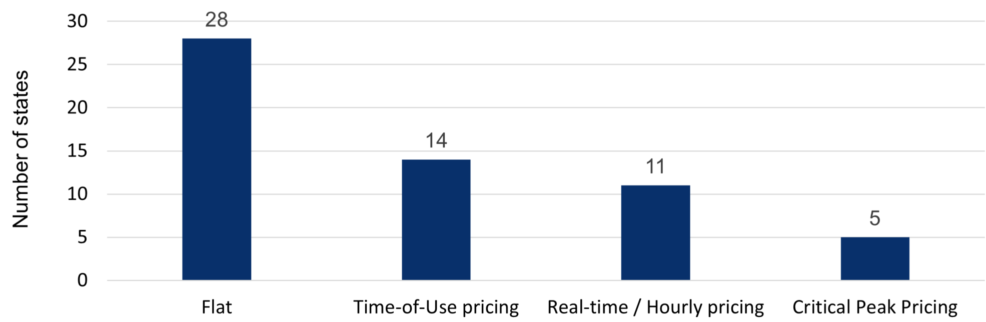


Figure 3.2.: Types of electricity tariffs available in the 27 EU states and Norway in 2020 (European Union Agency for the Cooperation of Energy Regulators, 2021)

5 countries (compare Figure 3.2). In the USA, 322 utilities (i.e. 34.89%) offer TOU tariffs for residential customers, 33 (3.58%) offer RTP tariffs, and 42 (4.56%) offer tariffs with peak pricing (U.S. Energy Information Administration, 2021).[6] Among those are large ones like San Diego Gas & Electric Co. (with 1,017,718 customers enrolled), Pacific Gas & Electric Co. (731,254 customers), and Ohio Power Co. (723,452 customers) (U.S. Energy Information Administration, 2021).

With respect to the technical properties of electricity, tariffs can specify the energy source (e.g. renewable electricity), the location of generation (e.g. regional generation or a specific individual generation plant), and power quality (e.g. commercial or industrial customers that require a certain sensitive voltage interval) (Salah et al., 2017; European Union Agency for the Cooperation of Energy Regulators, 2021).

Regarding risk allocation, tariff contracts determine if and how retailers or third parties are allowed to reduce, interrupt, or shift electricity delivery (Salah et al., 2017).

Regarding add-on products and services, today, electricity tariffs are oftentimes sold together with tariffs for water, natural gas, heating oil, wood pellets, and district heating (Bundesnetzagentur and Bundeskartellamt, 2021). In the future, tariffs can come with additional metering and communication devices, energy technologies, and related services. This represents a big trend, as the interviews with the retail market experts reveal. The experts expect that in the upcoming years, more and more retailers will offer not only tariffs, but also additional energy products and services.

[6]Peak pricing here includes Variable Peak Pricing, Critical Peak Pricing, and Critical Peak Time Rebate tariffs.

14 out of 15 interviewed experts see high or very high potential for cross-selling. For cross-selling, the experts name energy related hardware products, such as smart meters, PV plants, BEVs, heat pumps, batteries, wallboxes for BEVs, combined heat and power plants, non-energy hardware products such as household devices, telecommunication devices, and tickets for events, as well as services payment solutions for public BEV charging, device maintenance, and other add-on energy services. This hints at the emergence of new potential for customers to optimize switching of tariff together with residential energy technologies.

Furthermore, tariffs can be differentiated by medium of communication between customers and retailers (e.g. purely digital bills and online customer service), and give-aways such as monetary sign-up bonuses, or vouchers for other products.

The most frequently offered tariff type in Europe is a Flat, online, 100% green tariff that offers a give-away such as a sign-up bonus (European Union Agency for the Cooperation of Energy Regulators, 2021). This is mirrored by the statements of the interviewed experts. Asked about their impression on tariff characteristics that are important to the customers, the most frequently mentioned factors were transparency and understandability (9 mentions), simplicity (7), price guarantee (6), the origin and source of electricity (5), and the quality of service and the digital customer experience (5). Further mentions are contracts that are short and flexibly terminable (4), trust and fair treatment (3), available cooperations with hardware suppliers (1), customized tariffs (1), volume and frequency of pre-payments (3), and data security (1).

As a specialty of some retail markets' micro structure, there is a default allocation, meaning that customers have a default tariff assigned to them based on their location ("Grundversorgung"). This default takes effect, e.g. when customers move, or when customers cannot find another retailer willing to supply them (e.g. due to their credit history) and ensures that every citizen has access to electricity. However, these default tariffs from the primary suppliers are often more expensive. In Germany, residential customers supplied with the default tariff paid on average 33.80 ct/kWh in 2021, whereas they paid 31.89 ct/kWh for non-default tariffs from the primary supplier, and 32.70 ct/kWh for tariffs from other retailers (Bundesnetzagentur and Bundeskartellamt, 2021). Hence, residential customers with an annual consumption of 3,500 kWh, who are currently supplied under a default tariff could save about 67 Euro per year on average by switching their tariff (Bundesnetzagentur and Bundeskartellamt, 2021). Some retail experts claim that default tariffs are overpriced (Experts 6 and 13). To lower prices in default tariffs, two experts propose changes to this aspect of the current micro structure of retail markets: Either, primary suppliers could be randomly assigned to customers from a pool of retailers (Expert 10), or the role could be auctioned off every five years (Expert 13).

3.2.4 Business structure

The business structure comprises the business model and the pricing model, as well as explicit transaction costs (such as trading fees in auctions) (Dauer et al., 2017). In the context of retail markets, this typically includes the revenue margin, sign-up fees or bonuses, termination fees, and commissions that retailers pay to comparison platforms, switching service providers, and partnering companies for bringing in customers.

Since historically, retailers only sold the homogeneous product electricity, many retailers aim for price leadership and use sign-up bonuses as a key measure. In Germany, the average sign-up bonus in 2020 was 56 Euro for a non-default tariff contract with the primary supplier and 70 Euro for a tariff contract with another retailer (Bundesnetzagentur and Bundeskartellamt, 2021). Some retailers would deliberately offer high sign-up bonuses and later increase prices to improve their margins, hoping that customers would not switch again, says one interviewed expert (Expert 5). However, some experts see a convergence, where too many retailers aim for price leadership (Expert 12) and some customers have learnt to switch regularly to take advantage of high bonuses (Expert 5, 8, 12). The intensive level of price competition might be one of the key reasons why numerous retailers filed for bankruptcy during the wholesale price rally in late 2021 (Groeneveld, 2022).

Termination fees are forbidden in many European countries by law, except for very specific cases. For example, in Germany, a non energy specific law applies that forbids companies to include contractual penalties for the termination of a contract in their terms and conditions. Only in the case of an early termination of the contract before the end of the duration period specified in the contract, it may be legal to charge the resulting "damages" to the consumers (European Union Agency for the Cooperation of Energy Regulators, 2021).

For most retailers, partnerships with other companies play a big role for sales (Expert 1, 2) and are expected to further gain importance (Expert 4, 9, 11, 12, 13, 15). Types of partners include hardware providers for smart meters, solar PV plants, or mobility (Expert 1, 2, 4, 12), but also sales partnerships with cinemas, sustainable supermarkets, sports clubs, and public transport companies (Expert 6, 9), as well as energy service providers for energy efficiency certification, insurance etc. (Expert 11). Other retailers report that they have partnerships, and currently see limited direct impact on sales (Expert 5, 6), but a high impact on reputation building (Expert 5). This indicates that commissions might become increasingly important as the number of partnerships for retailers will rise.

3.2.5 IT infrastructure

The retail market's IT infrastructure contains the hardware and software that is required in order for markets to function on a technical level (Dauer et al., 2017). It plays a crucial role in the retail market, as many retailers and comparison platform providers interact with their prospective customers digitally – either partly (Expert 2, 3, 4, 5, 6, 9, 11, 14), or exclusively (7, 10, 15).

For the selection of tariffs, web portals and mobile applications are needed (Dauer et al. (2017), Expert 2). In terms of software, this requires, amongst others, data bases of offered tariffs (both for retailers and for platforms) and payment applications. In terms of hardware, this requires (web) servers and consumer end devices (computers, smart phones).

Once tariffs are selected, IT infrastructure is needed for metering and communication between retailer and customer. For instance, smart meters, adequate communication protocols, encryption mechanisms and firewalls are needed to ensure reliable system operation (Dauer et al., 2017).

Notably, standards for hardware and software can support the integration of different devices and technologies (Dauer et al., 2017). However, too strict certification processes can also slow down the adoption of new technologies, as the example of the German smart meter roll-out demonstrates (see Subsection 3.2.1).

3.2.6 Agent behavior

Agent behavior addresses the interaction of sellers and buyers on the market and results in the market outcome. The agents in this context are retail companies and residential, commercial, and small and medium industrial electricity customers. The participation of residential customers in the market can be most directly seen in their supplier switching behavior (European Union Agency for the Cooperation of Energy Regulators, 2021). Cramton (2017) proclaims that "most retail customers are poor electricity shoppers". However, it seems relevant to assess if customers can generally be simply divided into "good" and "poor" customers. To assess the heterogeneity of customer agents on the retail market in more detail, stakeholders were asked into which archetypes customers can be categorized according to their experience. The interviewed experts offer the following classifications:

- The non-switchers, and the switchers
- The non-switchers, the self-switchers, and the assisted switchers
- The technology-oriented, the ecologically oriented, the parsimonious, and the inert mass
- The parsimonious professionals ("price hoppers"), the ecologically oriented, the loyal price optimizers (i.e. internal switchers), the passive customers on default tariffs, the 'switchers by chance' (for whom switching is done by price concerned relatives, or who switch spontaneously at public retailer sales booths)
- A range between extreme price hoppers and loyal customers
- The bonus hoppers, the unhurried customers, and the sleepers
- The lazy, ignorant, and careless ones, the parsimonious, and the smart ones
- The eco purists, the frequent switchers, and the careless ones
- The non-switchers on default tariffs, the solid switchers, and the bonus hoppers

From these answers it can be derived that a variety of agent types exists. These answers also mirror some of the aspects that customers were reported to value in a tariff, as described in Chapter 3.2.3, as simplicity, price guarantees, source of energy, and short contracts. Moreover, they hint at additional aspects that different customers value, such as low prices, high sign-up bonuses, low switching effort, technological innovation, loyalty and reliability.

This can lead to very heterogeneous behavior of agents on the market. For market engineers that aim to improve efficiency of the retail market (by increasing switching rates), this finding indicates that there might not be one single reason for customers (not) to switch, but actually, a variety of reasons that take effect. As Schneider and Sunstein (2017) comment, the switching decision might for example be affected by behavioral inertia, by a sheer lack of information, the urge for simplicity, or by a (perceived) bad cost/benefit ratio. In order to switch away from their current tariff, consumers must gather information, weigh numerous tariff options, and fill out contracts. In addition, humans often "perceive a default to be the recommended option", especially when they are "unfamiliar with the respective context" (Schneider and Sunstein, 2017).

To this end, tariff recommendation tools appear as a key mechanism for reducing biases and transaction costs, and thus facilitating tariff switching. An interviewed customer rights agency confirms this, stating that transaction costs would certainly influence the probability and frequency of switching, and that comparison tools can help reduce transaction costs by reducing search costs. Therefore, that customer rights agency generally encourages customers to use such tools. However, existing comparison tools seem insufficient, as the majority of customers are not using them (compare Chapter 3.2.7), they rarely include dynamic tariff offers, and seem not to substantially simplify tariff comparison (European Union Agency for the Cooperation of Energy Regulators, 2021). Moreover, current implementations of such tools lead to new problems, as they do not always present tariffs in a consumer-friendly way. For example, if many settings have to be set up by the platform user, the complexity of switching can still be high. Moreover, if tariff advertisements are displayed above the actual search results, disguised as a very good search result, this can mislead consumers (Expert 13).

In summary, tariff recommendation tools seem to be desperately needed, but current implementations are not fully adequate and sufficient to motivate large shares of residential customers to switch, and moreover switch to system-beneficial time-varying tariffs.

3.2.7 Market outcome

The market outcome constitutes the result of the market's economic and legal environment, its market structure and the agent behavior. It can be measured by various indicators and enables evaluation and comparison of markets. For this thesis, electricity retail markets are evaluated regarding their competitiveness and efficiency. High competitiveness and efficiency are thereby characterized by three indicators, namely a high number of participants, low market concentration and power, and a high rate of transactions, i.e. switching of supplier.

Number of retailers

In European electricity retail markets, the number of nationwide participating retail companies varies strongly by country. Most retailers exist in Spain and Italy, with 292, and 175 active nationwide suppliers, respectively. On average, 47 nationwide retailers of electricity exist in EU countries. In most countries, the number of retailers has increased from 2019 to 2020. Exceptions are, e.g. Great Britain, and Finland (European Union Agency for the Cooperation of Energy Regulators, 2021). In Germany, customers could on average choose from 162 retailers (142 for residential customers) per grid area in 2020, a small increase from 156 (138) in 2019 (Bundesnetzagentur and Bundeskartellamt, 2021). The number of retailers therefore indicates sufficient competition in the German retail market. This is also the opinion of one interviewed customer rights agency that explicitly proclaims that there is a sufficient number of retail companies (Expert 13). However, only three retailers offer tariffs with dynamic pricing (Bundesnetzagentur and Bundeskartellamt, 2021).

Market concentration and market power

One relevant metric for market performance is the degree of market concentration. Low market concentration is generally desirable, as it limits the ability of single actors to exercise market power, and encourages innovation and good customer service

(European Union Agency for the Cooperation of Energy Regulators, 2021). Two common measures for market concentration are the Herfindahl-Hirschman Index (HHI) and the Concentration Ratio (CR).

The HHI equals the sum of the squared market shares of all market participants, multiplied by 100 (Rhoades, 1993). In the electricity retail market, the market share of a company can be regarded as the number of that company's electricity metering points, divided by all metering points in the residential electricity retail market. The European Union Agency for the Cooperation of Energy Regulators (2021) defines an HHI above 2,000 as an indicator for a highly concentrated market. As of 2020, one third of European states had low concentration levels, and two thirds had high concentration levels. In most countries, the HHI has decreased between 2018 and 2020. Especially high HHI values are observed in Latvia, Hungary, and Luxemburg. The HHI is lowest in the Nordic countries Norway, Sweden, and Finland.

Another common measure is the CP, the sum of the market shares of the largest companies in the respective market. For example, CP3 stands for the aggregated market share of the three largest companies in a market. In Europe, the CP3 varies between 38 and 100 depending on the country and is generally highly correlated with the HHI. In Germany, the CP4 is reported by the Bundesnetzagentur and Bundeskartellamt (2021). In 2020, the CP4 was 42.8%, indicating some, but no extreme market concentration. The Bundesnetzagentur and Bundeskartellamt (2021) proclaims that no single retailer has a dominant market position.

Furthermore, one interviewed retailer proclaims explicitly that they did not see any signs of cartels (Expert 6).

Switching rates

The annual switching rate of consumers is another important indicator of efficiently functioning retail markets. In Europe, switching rates differ strongly between countries. In 2020, the highest ("external") retailer switching rates, i.e. 21%, existed in Belgium and Norway. The lowest external switching rates could be observed in Hungary (0.2%) and Poland (0.7%) (European Union Agency for the Cooperation of Energy Regulators, 2021). This indicates that there is still large potential for increasing switching rates and thus the efficiency of the retail markets in Europe. In

Germany, 62% of customers are still with their primary supplier (Bundesnetzagentur and Bundeskartellamt, 2021).

Internal switching rates, i.e. the share of customers switching from one tariff to another tariff offered by the same retailer, can differ from external rates, and range from 0.9% in Luxembourg to 25.2% in Romania. Overall, switching rates tend to be higher among consumers with higher electricity consumption (European Union Agency for the Cooperation of Energy Regulators, 2021). This might hint at the fact that higher financial savings potential motivates more customers to switch. While in some countries, switching rates rose from 2019 to 2020, in others, rates declined. No overall European trend can be observed (European Union Agency for the Cooperation of Energy Regulators, 2021).

In Germany, 10.9% of residential customers switched their retailer in 2020, an increase of one percentage point, compared to 2019. Another 3.6% of customers switched to a new tariff, but stayed with their retailer (Bundesnetzagentur and Bundeskartellamt, 2021). Still, a majority of electricity is consumed via tariffs from the primary supplier - 25% from the default tariff and another 37% from other tariffs offered by the primary supplier (Bundesnetzagentur and Bundeskartellamt, 2021).

Interestingly, the interviewed experts see a generally well functioning retail market (Expert 13), with high competition and low margins (Expert 9). However, multiple experts note one big exception. That exception concerns primary suppliers who still have many customers, despite above-average pricing. One retailer contemplates that this might be because some customers are too lazy to switch or do not want to occupy themselves with the task of switching (Expert 6). One customer rights agency mentions that this is to the customers' own disadvantage, as default tariffs are oftentimes overpriced (Expert 13). To increase competition, the primary supplier role could be auctioned off, or randomly assigned from a pool of retailers in fixed time intervals (Expert 10, Expert 13). This could increase competition among retailers for customers, who are on default tariffs and improve the overall efficiency of the market.

3.3 Summary

Summing up the results of Chapter 3, five key points become evident. First, due to the uniform pricing wholesale market design in Germany and many other European countries, end-consumer electricity tariffs do not contain spatially differentiated energy price components, which can have negative effects on grid congestion and costs. Second, retailers need to innovate and diversify their business models, e.g. through cross-selling, as the retail market is highly competitive and mere price competition with low margins currently drives bankruptcies. Third, there is a prevailing lack of time-varying tariff offers for residential customers. Fourth, residential customers need to be better supported in switching tariffs and retailers. For this, new kinds of recommendation tools are needed, as existing tools are often insufficient. Fifth, once tariffs are adopted, continuous engagement of customers, e.g. through automated response to price signals, is needed in order to unlock the potential of consumer-centric electricity markets, as envisioned by the EU. These insights motivate the development of new solutions that make it easier for customers to switch to and use time-varying tariffs, as well as create new business opportunities for retailers based on time-varying tariffs. Such solutions are presented in Part II. The role of spatial tariffs in integrated energy systems is later investigated in Part III. The subsequent Chapter 4 presents the theoretical foundations of electricity tariffs and further establishes the benefits of tariffs that vary temporally, and spatially.

CHAPTER 4

ELECTRICITY TARIFF ENGINEERING

An electricity tariff can be defined as a set of rules that defines how individual customers are charged for their electricity consumption. I define *electricity tariff engineering* as the continuous process of analyzing and (re-)designing electricity tariffs and tariff related products and services with the objective of aligning the interests of electricity consumers, retailers, and society in a way that increases the economic efficiency, sustainability, and security of supply of the energy system.

From the system point of view, the tariff is the mechanism that decides how electricity system costs are distributed amongst all users that are connected to the system. There are multiple types of costs that have to be recovered. Typically, five cost categories can be differentiated: Energy costs (for electricity generation, capacity and ancillary services), network costs (for transmission and distribution grids), charges and levies for renewable energy subsidies, other energy related taxes and charges, and value added tax (European Union Agency for the Cooperation of Energy Regulators, 2021).

In many countries, e.g. most countries in Europe, the energy costs category makes up the largest share in residential electricity tariffs (European Union Agency for the Cooperation of Energy Regulators, 2021; Pérez-Arriaga and Knittle, 2016). In liberalized retail markets, energy costs are the one category that varies from retailer to retailer, and thus is the one category that customers can influence by switching to a different retailer.

For these two reasons, this thesis focuses primarily on energy costs.[7] Energy costs in general fluctuate over time and space because of changes in marginal power generation, the physical laws of electric flows in transmission and distribution grids, and the technical requirement of balancing electricity supply and demand at all times and locations (Schweppe et al., 1988). The economically efficient energy price can be defined as the short run marginal value of electricity at a given location at a given time, adjusted for network losses, congestion, and the potential for scarcity. These so-called Locational Marginal Prices (also known as nodal prices) reflect variations of the value of the marginal unit of electricity at different times and locations that are caused by changes in demand and supply, and the physical layout of the grid. If these prices are not passed on to consumers, but instead blurred in a linear ("Flat") per-kWh charge, the outcome will be economically inefficient (Joskow, 2007). While more beneficial outcomes can be achieved by tariff designs employing LMPs, they have some drawbacks, as they are complex to calculate, contain increased risks for investors, and face political opposition. Therefore, nodal prices historically have often been approximated by uniform or zonal time-varying tariffs, in the form of RTP, TOU, and CPP. Notwithstanding the lacking spatial granularity, those time-varying tariffs can considerably improve economic efficiency compared to Flat tariffs, by incentivizing customers to adjust their consumption in a system-benefiting way, based on the prices they see (Burger et al., 2020; Burger, 2019). For example, higher prices during certain times can motivate customers to reduce their demand (Faruqui et al., 2017), thus reducing the system peak and capacity costs (Faruqui et al., 2010). In the following paragraphs, these three most common types of time-varying tariffs are characterized.

In contrast to a Flat tariff, in which the energy price is constant, *Time of Use tariffs* have energy prices which vary by time of day, and in some cases by weekday or season (European Union Agency for the Cooperation of Energy Regulators, 2021). TOU tariffs are proxies of the more granular RTP, as they typically have fewer price variations. The second key difference is that unlike RTP tariffs, TOU prices are set in advance, with no further real time adjustment. Once prices have been determined,

[7]For two recent dissertations with a focus on other cost categories, the interested reader is referred to Burger (2019) and Schittekatte (2019).

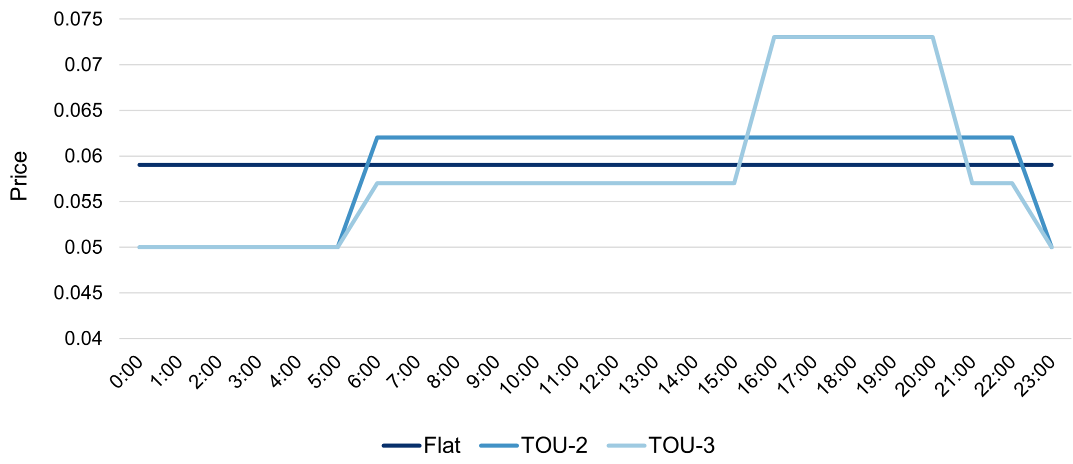


Figure 4.1.: Archetypal Flat tariff and TOU tariffs

they are valid for a longer period of time, until the regulator chooses to review them (Faruqui and Palmer, 2011). On the one hand, the a priori fixing and the lower temporal granularity decrease economic efficiency (Borenstein, 2005). On the other hand, these characteristics lead to TOU tariffs being perceived as simpler and less risky than RTP and CPP (Faruqui and Palmer, 2011). Another benefit of the TOU tariff is that it can be implemented with less complex information and communication technology. These might be reasons why TOU tariffs are the most widely used of all time-varying tariffs. In some European countries, such as Italy, Croatia and the Netherlands, the majority of residential customers are using a TOU tariff (European Union Agency for the Cooperation of Energy Regulators, 2016). Figure 4.1 shows a typical example of two TOU tariffs - one with two (TOU-2), and one with three different price periods within a day (TOU-3). In general, TOU tariffs with any number of price levels could be implemented, but a limited number of price levels maintains a certain simplicity and understandability.

Unlike TOU tariffs, *Real-time pricing tariffs* are typically derived directly from wholesale energy prices and thus change every 15 - 60 minutes (see Chapter 3). Figure 4.2 shows an exemplary RTP tariff with an hourly resolution. RTP tariffs send more economical efficient tariff signals than TOU, CPP, and Flat tariffs, because they better reflect the actual wholesale electricity prices. In fact, for the PJM mar-

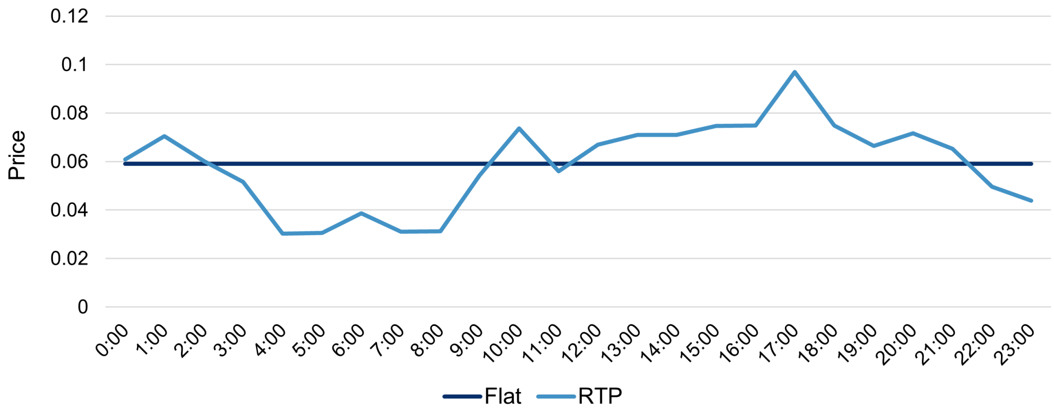


Figure 4.2.: Archetypal Flat tariff and RTP tariff

ket in the US, Hogan (2014) found a "substantial difference in efficiency between even the best TOU design and RTP". However, human behavioral biases can affect actual electricity consumption decisions. Inattention, decision fatigue, present bias or hidden costs could lead to customers not responding to RTPs as neo-classical economics would expect (Schneider and Sunstein, 2017). Besides, transaction costs (e.g. for smart meters, or for planning ahead and manually turning on household appliances in times of low prices) can be higher than the resulting savings. Since TOU tariffs have less volatile prices and price levels are fixed for typically at least a year, they can actually lead to similar, or even higher economic efficiency in practice, under some assumptions (Schneider and Sunstein, 2017).

Critical peak pricing tariffs commonly use a baseline Flat, or TOU energy price in combination with peak prices during extremely critical periods (Hu et al., 2015; Burger et al., 2020). Those peak prices are typically announced on short notice, e.g. 24 hours ahead of the critical event period. Critical periods only occur a few times per year and prices can be "several multiples" of the off-peak price (Faruqui et al., 2017). Figure 4.3 exemplifies a CPP structure in which a peak price is set at 5-7pm on a peak event day, with a peak to off-peak ratio of 5. Since peak prices lead to higher revenues for the utility during critical hours, the price for the rest of the hours is typically lower than on a standard Flat tariff (Burger et al., 2020). CPP tariffs give especially strong incentives for demand reduction in critical hours. They typically induce a larger demand response from residential customers than TOU tariffs. Faruqui et al. (2017) perform a meta-analysis of 63 dynamic pricing pilots

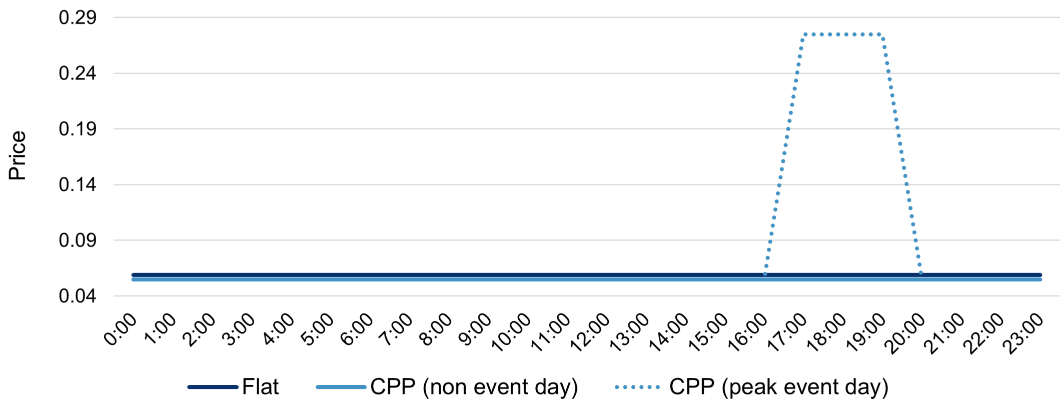


Figure 4.3.: Archetypal Flat tariff and CPP tariff

from nine countries on four continents. They find that peak reduction increases with the peak to off-peak ratio. During peak events, CPP tariffs have a significantly higher peak to off-peak ratio than TOU tariffs. This can lead to overall greater demand adjustments, bill changes and socio-economic impacts.

To summarize, Figure 4.4 displays the design options for electricity tariffs, regarding their temporal and spatial granularity. Whereas the spatial dimension is typically subject to central regulatory decisions, the decision about temporal granularity is – within regulatory limitations – up to retailers and consumers in liberalized retail markets. In the spatial dimension, design options are single-zone prices, multi-zone prices, and nodal prices. In the temporal dimension, design options are flat, invariant prices, time-of-use prices, critical peak prices, and real-time prices. This thesis addresses both dimensions, i.e. the temporal dimension in Part II, and the spatial dimension in Part III.

Past tariff design research has robustly established the theoretical efficiency benefits of higher temporal and spatial granularity of the energy components in electricity tariffs, compared to prevailing Uniform Flat tariffs. Moreover, empirical studies have confirmed that consumers have positive price elasticities and that a widespread use of economically efficient tariffs has system-beneficial effects.

Yet, the status quo review in Chapter 3 uncovers that this potential is not captured in practice. This calls for new solutions in the field of electricity tariff engineering. Tariffs and tariff related tools need to be updated to better align the interests of

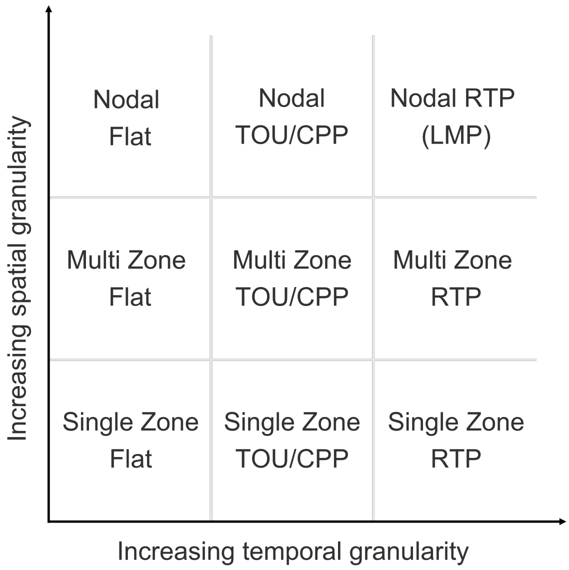


Figure 4.4.: Design options for the energy component of electricity tariffs

electricity consumers, retailers, and society in integrated energy system and unlock their great potential regarding societal costs, sustainability, and security of supply. To facilitate the proliferation and use of time-varying tariffs, the customer-focused Part II of this thesis develops tools that foster adoption of such tariffs, and tariff based demand response.

Part II.

Customer Level

INTRODUCTION TO PART II

As outlined in Part I, residential customers are becoming a more important part of the electricity system due to the electrification of private energy consumption, which further increases the importance of electricity tariffs to steer system-efficient consumption. The proliferation of innovative, economically efficient tariffs for residential customers can yield considerable system benefits (see Chapter 4). However, in liberalized electricity retail markets, tariffs are selected by the individual customer, and adoption rates of time-varying tariffs and smart meters are still low (see Chapter 3).

Hence, it is important to research methods, which enable residential customers to select system-beneficial time-varying tariffs, which are also beneficial for the customers themselves. In Part II, I develop decision support tools for tariff selection (Chapter 5), and for tariff-technology bundle selection (Chapter 6). I also model optimized automated demand response to tariffs (Chapter 6) and develop net load forecasting models that can serve as inputs for such optimization (Chapter 7 and 8).

CHAPTER 5

ASSESSING THE ECONOMICS OF RESIDENTIAL ELECTRICITY TARIFF SELECTION

In this chapter, I assess the economic potential of tariff switching for residential consumers and evaluate a naive method for selecting the cost-minimal tariff. For this, I design a set of five time-varying tariffs and one benchmark Flat tariff. By applying these tariffs to one-year consumption time series data of more than 100,000 customers, I calculate the electricity bills of customers under the different tariffs. I find that for the majority of customers, bill variations are small, but for a small number of customers, bills vary considerably. Furthermore, I propose a naive tariff selection approach based on individual consumption data of one month. Finally, I assess the economic consequences of selecting a sub-optimal tariff.

This chapter comprises the published article: F. vom Scheidt, P. Staudt, C. Weinhardt, *Assessing the Economics of Residential Electricity Tariff Selection*, 2019 International Conference on Smart Energy Systems and Technologies (SEST), 2019.

5.1 Introduction

The transformation of the European electricity sector increases the importance of residential electricity tariffs -– the prices and charges that residential customers pay for consuming electricity. In the course of its *Clean Energy For All Europeans* package, the EU sets out to strengthen the role of consumers within an increasingly decentralized system (European Commission, 2016). As part of this, EU legislation requires electricity providers to offer more time-varying tariff options for residential customers (de Clercq, 2018; Bundesministerium für Wirtschaft und Energie, 2019). Simultaneously, current improvements and cost-decreases in advanced metering infrastructure and communication technologies permit real-time metering, price communication and demand response, thus enabling the effective implementation of new residential tariffs. In the EU, it is estimated that as of 2020, 123 million smart meters were installed, corresponding to a share of 43% of electricity consumers (European Union Agency for the Cooperation of Energy Regulators, 2021).

It has been shown that when confronted with efficient time-varying price signals, households adapt and consume electricity in a more system-beneficial way (Faruqui et al., 2017, 2010). Large scale application of time-varying tariffs holds the potential to reduce system costs by several billion Euros in the EU (Faruqui et al., 2010). Thus, the introduction of new, economically efficient electricity tariffs for residential customers can make a significant contribution to the transformation of the European energy system. However, while system benefits are positive, each individual household's private benefit or loss highly depends on the household's consumption profile and the respective tariff. An increasing number of households in the EU is equipped with digital electricity meters allowing consumption measurements in real-time (European Commission, 2018). Alas, in locations where households are free to choose whether to install a smart meter or not, like Germany and Portugal, installation rates are oftentimes low (European Commission, 2014). Moreover, in locations where smart meter adoption is mandatory, time-varying tariffs are often still unpopular (Hu et al., 2015; European Union Agency for the Cooperation of Energy Regulators, 2016; U.S. Energy Information Administration, 2021). This shows the need for new methods to support consumers in their tariff selection process.

Several studies on tariff recommendation and selection exist. Ramchurn et al. (2013) introduce an agent based platform for simulating electricity tariff selection. The platform forecasts hourly electricity consumption and makes load shifting recommendations based on individual loads of households. The authors use a Gaussian process, which combines both long-term consumption data of an average household and short-term consumption of the individual household. The model is evaluated on a consumption data set of 18 households. Results show that the model slightly outperforms two naive benchmarks. The study mentions that the model could be useful for identifying saving opportunities from time-varying tariffs, but does not explicitly calculate those.

Fischer et al. (2013) use the same model and find that in a small sample of ten households, annual savings between £35 and £391 can be achieved by switching from a Flat to the cheapest TOU tariff. Savings are predicted based on a three-month data sample. User interviews indicate that reliability of the recommendations is a big concern for the participants. This further motivates assessing the reliability of tariff recommendations in our study.

Ericson (2011) address some retailers' concern that time-varying tariffs may induce self-selection of consumers who benefit only because they have a well-fitting consumption pattern, and not because they change their consumption behavior in a system-benefiting manner. The authors model tariff selection as a function of compensating welfare measures. The study examines self-selection of customers into a CPP tariff. The findings indicate that consumption patterns have no significant influence on selection of the CPP tariff, but customers with higher flexibility are more inclined to select it. The authors also suggest that informing customers about the cost saving potentials of new tariffs may lead to an increased self-selection of price responsive households. This supports the motivation of our work, which is to quantify the economic risks and opportunities of tariff selections.

Luo et al. (2019) propose an electricity tariff recommender system for residential customers. From each customer's data, key electricity consumption features are extracted. Then, customers with similar features are identified. Last, a tariff is recommended to each customer, based on the tariff choices of customers with similar features. The classification method does not consider individual bills, but works with several simplifications, such as: "Users with large seasonal energy consumption deviations would prefer to choose the fixed rate plan; otherwise, the users would prefer the variable rate plan." The model is evaluated on 1,000 customers and three tariffs. Results show that the model outperforms a naive benchmark.

In summary, the existing body of literature on one hand demonstrates the academic interest in the topic of tariff recommendation and selection, and on the other hand leaves ample space for further meaningful contributions regarding the development of concrete recommendation methods and evaluation metrics.

To address aforementioned issues, this chapter employs a uniquely large electricity consumption data set. We design six tariffs based on empirical data. Next, we calculate and analyze customers' bills under those tariffs, thus quantifying the potential individual economic consequences of tariff selection. Finally, we propose a naive solution for tariff selection under limited information and evaluate its performance statistically and economically. Thus, this chapter a) assesses the economic consequences of residential tariff selection and b) introduces and evaluates a benchmark method for tariff selection.

5.2 Data and Methods

The following subsections present the data set used and the tariffs designed for this case study. The nomenclature for all tariffs is displayed in Table 5.1.

5.2.1 Data

The residential electricity consumption data used in this case study is acquired from Commonwealth Edison (hereafter: ComEd). ComEd is one of the biggest electric utilities in the United States of America, serving over four million customers in the state of Illinois (Exelon, 2018). The data set contains the anonymized electricity consumption data of 100,170 residential customers for the entire year of 2016. The electricity consumption is measured with smart meters and reported in 30-minute intervals. A detailed description of the data set and preprocessing is given in Burger et al. (2019).

One of the key principles in tariff design is full cost recovery (Bonbright, 1961). This means that the retailer should be able to recover all its costs through its tariffs. In order to ensure full cost recovery and to achieve realistic results, we design all tariffs in this chapter to be revenue neutral compared to the existing ComEd default tariff. Vertically unbundled utilities who act as electricity retailers can only influence one component of a tariff directly: the *energy costs*, which include all costs for procuring electricity. For ComEd's residential customers, the energy related costs account for 41% of total costs. All other tariff components are determined in a regulatory process (e.g. grid fees) or relative to other components (e.g. electricity taxes). In this chapter the latter two categories are intentionally kept the same under all tariffs, because the retailer cannot influence them directly. For energy costs, which can be influenced by the retailer, this chapter explores three different allocation methods, namely Flat, TOU, and RTP.

5.2.2 Flat tariff

Flat tariffs are the most common residential tariff design in many countries (see Section 3.2). The Flat tariff that we design for this case study is an exact replica of the actual Flat tariff from the ComEd territory. It allocates energy costs via an invariant, volumetric $/kWh charge. 95.8% of ComEd's residential customers were served under this tariff in 2016.

5.2.3 Time-of-Use tariff

TOU tariffs employ prices, which are set in advance with no further real-time adjustment. In Europe, TOU is by far the most widespread version of time-varying tariffs (see Section 3.2). Opting for a design similar to practice, a three level TOU design is designed for this case study (TOU-3). Results of TOU tariff calculations are naturally sensitive to the selection of time periods and price levels during those time periods. To account for some of this sensitivity, we consider three possible designs of a TOU-3 tariff. The TOU-3 energy prices are determined based on the annual average of the hourly load zone LMPs in the ComEd territory from 2016. These average hourly prices are depicted in Figure 5.1 as black points. By averaging several of these hourly prices within a certain time period of the day, the TOU-3 energy prices are determined, depicted as colored lines in Figure 5.1. In between the three versions (TOU-3a, TOU-3b, and TOU-3c), the lengths of the three TOU-levels (base, shoulder and peak) are varied. Apart from the energy charges, the rest of the tariff remains unchanged compared to the Flat tariff. In line with all other tariffs in this chapter, each TOU tariff version is designed in a way that the same revenue as under the existing Flat tariff is recovered. To reach this goal, the initially calculated TOU price levels are multiplied by a common revenue factor rf. Thus, the ratio between the TOU price levels is kept constant. This approach follows related tariff studies (Borenstein, 2006, 2013). For the three TOU-3 versions, prices are determined based on the average price within each *level*, as stated in Equation 5.1, with real-time price RTP, hour h, and the revenue requirement factor rf.[8]

[8] rf is 1.77 for TOU-3a, 1.78 for TOU-3b, and 1.79 for TOU-3c respectively.

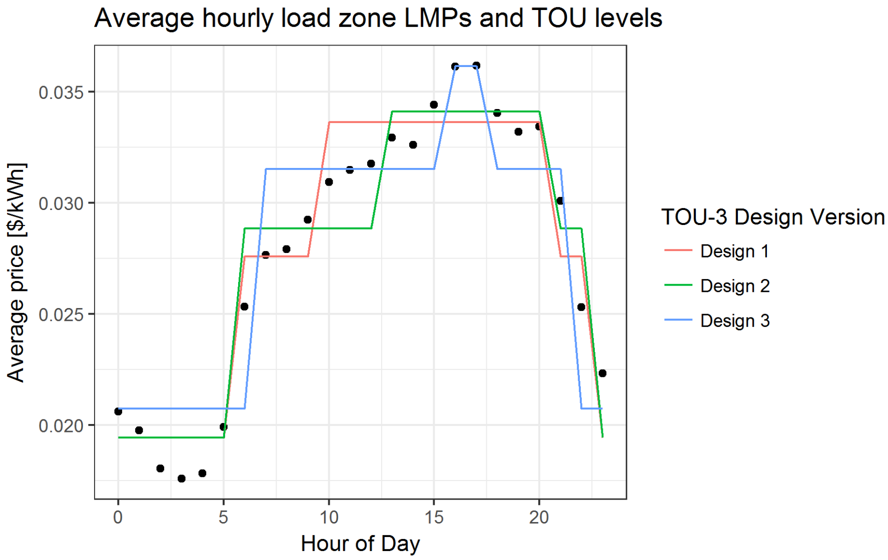


Figure 5.1.: Average hourly ComEd load zone LMPs in 2016 and derived 3-level TOU prices.

$$p_{TOU-3,level} = \frac{\sum_{h \in level}(\frac{\sum_{d=1}^{366} RTP_{h,d}}{366})}{|h|_{level}} \cdot rf \quad \forall level \in \{base, shoulder, peak\} \tag{5.1}$$

Note that with this design, TOU prices are the same on every day of the year. In addition to the TOU-3 tariffs, a 24-level TOU tariff (TOU-24) is designed. Here, for each single hour, the average RTP in a month is calculated and set as the respective energy price in that hour. Therefore, the TOU-24 prices change by hour, but are the same every day of a month. Again, hourly prices are adjusted in order to reach revenue neutrality. This is achieved by adding a fixed sum to the volumetric charge, as shown in Equation 5.2. Hence, the hourly TOU-24 energy price is defined by Equation 5.2, with RTP as the real-time price, H as the set of all hours h in a day, D as the set of all days d in a month, M as the set of all months m in a year, and the revenue requirement adder ra.[9]

$$p_{TOU-24,h,m} = \frac{\sum_{d \in D} RTP_{h,d}}{|D|_m} + ra \quad \forall d \in D, \forall h \in H, \forall m \in M \tag{5.2}$$

[9] ra is 0.02 \$/kWh for the TOU-24 tariff.

Table 5.1.: Nomenclature

p	energy price	$\$/kWh$
RTP	ComEd residential real-time price	$\$/kWh$
$\|h\|_{level}$	number of hours in price level	–
rf	revenue requirement factor	–
ra	revenue requirement adder	$\$/kWh$
h	hour	–
H	set of all hours h in a day	–
d	day	–
D	set of all days d in a month	–
m	month	–
M	set of all months m in a year	–

5.2.4 Real-time price tariff

RTP tariffs have seen less practical application than other time-varying tariffs (see Section 3.2). However, RTP tariffs represent a more economically efficient method of allocating energy costs than TOU, because they better reflect the marginal costs of generation and consumption of electricity (see Section 4). RTP tariffs thus promise the largest system benefits. Hence, adequately recommending their adoption is of high relevance. We base the price of the RTP tariff on the average of the hourly load zone LMPs in the ComEd territory. An exemplary price profile for one day can be seen in Figure 5.2.

To this price, a fixed factor is added in order to render the tariff revenue neutral, as noted in Equation 5.3. Note that unlike the TOU prices, the real-time prices change both by hour and by day. The energy price of the RTP tariff is defined in Equation 5.3 with real-time price RTP, hour h, and revenue adder ra.[10]

$$p_h = RTP_h + ra \tag{5.3}$$

5.2.5 Tariff selection method

Reliably forecasting a household's savings potential from switching to a time-varying tariff could incentivize self-selection into those tariffs. Since certain time-varying tariffs are only available with smart meters, such saving forecasts can in addition

[10] ra is 0.02 $/kWh for the RTP tariff.

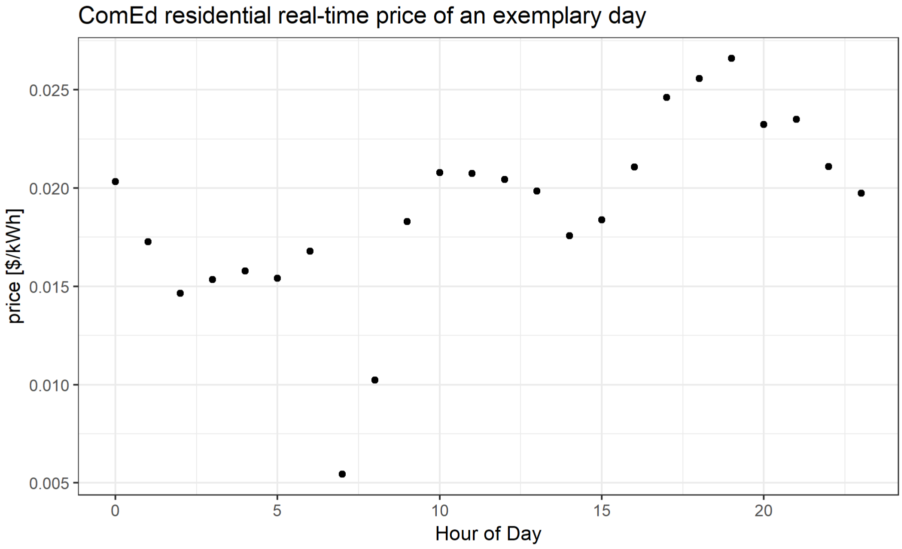


Figure 5.2.: The hourly load zone average LMP for the 24 hours of January 1st.

incentivize the adoption of smart meters. The limited availability of smart meters motivates exploring the question of how customers can make well-informed tariff selection decisions under limited consumption data availability. We propose using the electricity bill information of one month to determine the cheapest tariff. This requires high-resolution consumption data for one month. To get this data without smart meters, various inexpensive technologies can be used by customers or service providers. Existing solutions rely on webcams, which optically record readings from *analogue* electricity meters and optical character recognition software to extract the data (pixolus GmbH, 2019; Anyline GmbH, 2019). Data from simple *digital* meters can be accessed via commercially available infrared receivers. The scenario in this study is as follows: After recording consumption data for one month, the potential monthly bills under all available tariffs are calculated. The tariff, which yields the lowest monthly bill is recommended for selection. To assess the performance of this naive classification method, we subsequently calculate the customers' annual bills under all available tariffs and compare the results. Note that we repeat the classification for each of the twelve months and average the results for each household. We then average the results over all households.

5.3 Results

For this analysis, we are interested in the monthly and annual bills of residential customers under each of the six designed tariffs. Assuming no short-term demand response, we calculate the respective bills for each of the 100,170 households. Under the default Flat tariff, customers' annual expenditures range from \$141.14 to \$8,612.92. The mean annual bill is \$778.92.

5.3.1 Spread in electricity bills

Next, we quantify the potential individual economic impacts of the tariff selection decision. From the annual bills, we derive the spread between the most and the least expensive tariff option for each household. Note that the Flat tariff is included in this analysis. Both switching to a sub-optimal new tariff and staying with a sub-optimal (Flat) tariff yields unnecessary costs for customers.

For the majority of customers, only small annual bill differences are identified, as Figure 5.3 displays. In fact, over 90% of customers have a spread of less than \$25. For a small share of customers substantial absolute differences exist. 9,411 households (equivalent to 9.40%) have a spread above \$25. 3.58% (i.e. 3,586 households) have a spread of above \$50 and 1.73% (1,732) have a spread above \$100 per year.

5.3.2 Tariff selection

The calculated cost spreads show that identifying the cost-minimal tariff can yield substantial savings for certain customers. Table 5.2 presents the probabilities that a certain tariff is the cost-optimal tariff for a household, based on the yearly electricity bill. For most customers (52.38%), TOU-24 is optimal on a yearly basis (column "TOU-24", row "Total"). For 26.34% of customers, the default Flat tariff is cost-optimal. There are comparably fewer cases in which each TOU-3a, TOU-3b, and TOU-3c are optimal. This is presumably due to these three tariffs being fairly similar to each other. Besides, Table 5.2 also shows the instances in which a tariff is identified as cost-optimal based on the monthly measurement. For example, across

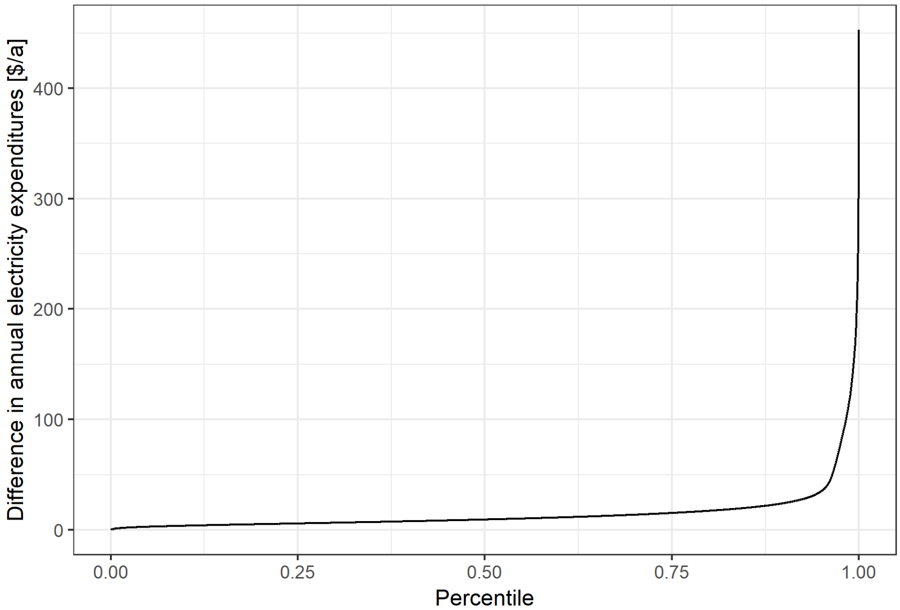


Figure 5.3.: Sorted maximum difference in annual electricity expenditures

all customers, RTP is the cost-optimal tariff in 38.22% of months (row "RTP", column "Total"). However, it is only the cost-optimal yearly option for 11.89% of customers. This indicates that when customers select a new tariff based on information from only one month, they are prone to select a tariff that is not cost-optimal on an annual basis. We refer to this as *tariff confusion*. As visible in Table 5.2, the probabilities of confusion vary strongly by tariff combination.

Table 5.2.: Probabilities of tariff confusion

	Cost-optimal annual tariff						
Cost-optimal monthly tariff	Flat	TOU-3a	TOU-3b	TOU-3c	TOU-24	RTP	Total
Flat	0.1435	0.0130	0.0076	0.0083	0.1930	0.0398	**0.4051**
TOU-3a	0.0006	0.0082	0.0005	0.0006	0.0303	0.0080	0.0482
TOU-3b	0.0024	0.0016	0.0026	0.0003	0.0266	0.0072	0.0408
TOU-3c	0.0027	0.0014	0.0002	0.0020	0.0140	0.0034	0.0238
TOU-24	0.0187	0.0066	0.0029	0.0022	0.0602	0.0092	0.0999
RTP	0.0954	0.0191	0.0085	0.0082	0.1996	0.0513	**0.3822**
Total	**0.2634**	0.0500	0.0223	0.0216	**0.5238**	0.1189	1.000

In order to further assess the naive classifier's performance across tariffs, we calculate precision (Equation 5.4) and recall (Equation 5.5). We define *True Positives* as all cases in which the tariff is correctly recommended by the method. *True Negatives* are all cases in which the method rightfully does not recommend a tariff. A *False Positive* describes a case in which a tariff is the cost-optimal monthly tariff (method recommends this tariff), but not the cost-optimal annual tariff (and therefore should not be recommended). A *False Negative* is defined as a case in which a tariff is not the cost-optimal monthly tariff (method does not recommend this tariff), but is the cost-optimal annual tariff (should be recommended).

$$Precision = \frac{\#TruePositives}{\#TruePositives + \#FalsePositives} \tag{5.4}$$

$$Recall = \frac{\#TruePositives}{\#TruePositives + \#FalseNegatives} \tag{5.5}$$

Table 5.3 displays precision and recall of choosing tariffs based on one month of information. TOU-24 has the highest precision of all tariffs, due to relatively few false positives (compare Table 5.2). Flat and RTP have the highest recall.

Table 5.3.: Results of monthly tariff recommendation

Tariff	**Precision**	**Recall**	**F1-score**
Flat	0.35	0.54	0.43
TOU-3a	0.17	0.16	0.17
TOU-3b	0.06	0.12	0.08
TOU-3c	0.09	0.09	0.09
TOU-24	0.60	0.11	0.19
RTP	0.13	0.43	0.20

From a customer's point of view, both precision and recall are important. High precision is desirable as falsely selecting a tariff could cause high costs. High recall is desirable as an undetected optimal tariff leads to missed saving opportunities. Therefore, we calculate the F1-score, which combines precision and recall as shown in Equation 5.6. The greater the F1-score, the better a classifier's performance. False positives and false negatives penalize the F1-score symmetrically.

$$F_1 = \frac{2 \cdot Recall \cdot Precision}{Recall + Precision} \tag{5.6}$$

Table 5.3 shows that while TOU-24 and RTP have very different precision (0.60 vs. 0.13) and recall (0.11 vs. 0.43), their F1-scores are similar. The Flat tariff has the highest F1-score (0.43). The three TOU-3 variants have the lowest F1-score. Together with the relatively high confusion values among these tariffs (compare Table 5.2, consider conditional probabilities), this result indicates that if a larger number

Table 5.4.: Median and 95%-quantile of costs of tariff confusion [$/kWh]

	Cost-optimal annual tariff					
Cost-optimal monthly tariff	Flat	TOU-3a	TOU-3b	TOU-3c	TOU-24	RTP
Flat	0.0 (0.0)	**7.4 (25.7)**	3.7 (15.3)	2.8 (12.2)	**4.6 (17.7)**	**8.7 (38.4)**
TOU3a	3.0 (10.6)	0.0 (0.0)	0.2 (1.1)	0.2 (1.1)	2.8 (9.5)	**4.2 (17.2)**
TOU3b	4.1 (12.9)	0.3 (1.5)	0.0 (0.0)	0.6 (2.2)	3.3 (11.0)	**4.5 (18.2)**
TOU3c	3.8 (12.1)	0.4 (1.9)	0.5 (2.1)	0.0 (0.0)	3.3 (10.8)	**4.8 (18.4)**
TOU24	**5.5 (18.7)**	1.3 (5.8)	1.3 (6.3)	1.6 (6.9)	0.0 (0.0)	0.4 (2.4)
RTP	**12.1 (29.2)**	5.3 (15.1)	**6.8 (17.5)**	**7.7 (17.6)**	2.5 (8.7)	0.0 (0.0)

of similar tariffs is available, selecting the optimal tariff becomes more difficult. In turn, we expect that the more similar tariffs are available, the lower the financial costs of tariff confusion. Therefore, in a final step, the economic consequences are analyzed. We calculate the costs of false positives and false negatives for each tariff. The median value as well as the 95%-quantile value are displayed in Table 5.4. For example, if the Flat tariff is selected, but the RTP tariff is the actual cost-optimal annual tariff, the median household affected by this case would face additional annual costs of $8.7, and the 95%-quantile household would experience additional annual costs of $38.4. This shows that the economic consequences of tariff selection vary substantially among households and tariffs. The results for TOU-3a, TOU-3b, and TOU-3c indicate that if more similar tariffs are available, costs of tariff confusion decrease.

5.4 Discussion

The findings in this chapter regarding total bill spread are subject to the following assumptions. First, we design all tariffs to be revenue neutral for the retailer, given the consumption profiles of all 100,170 customers. We do this to avoid an unbalanced data set in which all customers are better off by selecting one dominant tariff. In reality, retailers would not have this information a priori and therefore, additional saving opportunities for customers are likely. Second, the tariff analysis does not consider the effects of demand response and might therefore underestimate the benefits of time-varying tariffs. It is therefore worthwhile to simulate demand response in future studies to uncover the true potential of time-varying tariffs (see Chapter 6). Third, the validity of our findings can be improved by assessing data sets from other regions, and additional tariffs and input time periods.

5.5 Conclusion

This chapter contributes to the transformation of the electricity system by assessing the economic consequences of residential tariff selection. We quantify the savings potential for individual households. We find that for a share of the population tariff selection yields substantial economic consequences even under conservative assumptions. We present and evaluate an application-oriented approach for cost-optimal tariff selection based on bill information of one month. Results show that the performance of this naive classifier differs strongly between tariffs. The 24-level TOU tariff shows the highest precision. Highest recall is achieved for the Flat tariff, followed by the RTP tariff. We analyze costs of tariff confusion and find that the RTP tariff is especially prone to high costs through false selections. Moreover, our results indicate that availability of more similar tariffs decrease the performance of the tariff classifier, but also the costs of tariff confusion. The logical next step for research is therefore to use the methods and results of this chapter as a benchmark, and to develop more sophisticated tariff selection methods such as Machine Learning classification algorithms. Another interesting pathway for future research lays in behavioral experiments to assess under which circumstances customers follow recommendations.

This chapter shows that the performance of a naive recommendation method differs between tariffs. The TOU-24 tariff and RTP tariff have the highest confusion probabilities. For no tariff, the naive approach achieves a precision or recall higher than 60%, which can limit trust in the recommendation amongst consumers. This motivates the development of more complex methods to achieve higher tariff recommendation accuracies. Moreover, the results indicate that the economic consequences of the naive recommendations are small for most customers. The median annual extra costs for selecting sub-optimal tariffs are in the range of 0.2$ to 12.1$, depending on the recommended tariff. Wrongfully selecting the RTP tariff leads to the highest median extra costs. Importantly, the small size of economic consequences is not caused by the accuracy of the recommendations, but rather by the limited total difference in electric bills under different tariffs. This encourages future research, which expands tariff-only recommendations to recommendations of tariffs and associated residential energy technologies in one bundle, which might increase potential customer savings.

This chapter thus showcases the application of a basic method and fundamental metrics for individual tariff recommendation and uncovers two directions of promising future research. These directions are pursued in the subsequent Chapter 6.

CHAPTER 6

A RECOMMENDATION TOOL FOR TARIFF-TECHNOLOGY SERVICE BUNDLES

Electricity retailers in European markets often face strong price competition and lately the disruption of their conventional business model, i.e. selling electricity for a invariant price per kilowatt-hour, through increasing self-generation of their customers. However, the widespread uptake of technologies such as smart meters, rooftop solar PV plants, batteries, heat pumps, and electric vehicles by residential customers also represents the chance for retailers to diversify their portfolio and unlock new revenue streams. The major trends for companies in the retail market, as identified in Chapter 3, include simplifying tariff switching for customers, cross-selling of hardware, and servitization. To this end, this chapter presents a novel data-driven model and corresponding case study for the recommendation of service bundles of technologies and tariffs to residential customers, based on individual household characteristics.

The results reveal large saving potentials through such bundles, compared to tariff switching alone. Time-varying electricity tariffs make energy technologies more financially attractive for many customers, and likewise, flexible energy technologies make time-varying tariffs more financially attractive. In terms of recommendation accuracy, the developed Machine Learning recommendation models outperform a defined naive benchmark clearly. They also enable better savings for customers, on average. Finally, it is demonstrated that 'collaborative data', i.e. four week excerpts of smart meter data that the customers provide to the retailer, improve the mean accuracy of recommendations. In summary, this chapter thus presents multiple promising methodological and conceptual approaches for retailing time-varying electricity tariffs in integrated energy systems.

This chapter comprises the unpublished article: F. vom Scheidt, P. Staudt, *A Data-Driven Recommendation Tool for Sustainable Energy Service Bundles*, Working Paper, 2022.

6.1 Introduction

The worldwide transition of energy systems forces electricity retailers to fundamentally change their business model. The traditional business model relies to a large extend on selling electricity for an invariant per-kilowatt-hour (kWh) tariff. This model is disrupted by new competitors, and the proliferation of rooftop solar PV and home battery storage systems, with some scholars and practitioners projecting a "utility death spiral" (Pérez-Arriaga and Knittle, 2016). However, cost reductions in sustainable energy technologies like PV, battery storage, heat pumps (HPs), and BEVs, together with improvements in information and computation technology and novel time-varying tariffs also represent a chance for retail companies. They can enable retailers to diversify their product and service portfolio, thus differentiating their offer in a highly competitive market and unlocking new revenue opportunities (compare Chapter 3). For retail customers, tariff switching commonly comes at the cost of searching information, comparing offers, and filling out contracts. These costs are set-off by relatively small savings that can be achieved by tariff switching (see Gottwalt et al. (2011); Arora and Taylor (2016); Zhang et al. (2019); vom Scheidt et al. (2019) and Chapter 3 and 5). A bundle recommendation tool can decrease the switching costs and at the same time increase the potential savings for customers. In the big picture, this can lead to an increased adoption and use of system-beneficial time-varying electricity tariffs, smart meters, and electric technologies that substitute fossil fuel based heaters and cars. This can yield large societal benefits by reducing system costs and emissions (see Chapter 2 and 4). In summary, electricity retailers, their customers, and society as a whole could benefit strongly from the combined, optimized sales of tariff-technology bundles. This poses the challenge to design a corresponding recommendation tool for energy service bundles that unlocks reliable cost savings to customers and cross-selling opportunities for electricity retailers.

To this end, we present a novel Machine Learning classification model for recommending cost-minimal service bundles of technology leases and tariffs to residential customers. The model uses household characteristics and sparse historical data as inputs. The preceding labelling of the data set is done based on a smart home energy management system optimization. We apply this approach to a set of 292 households from London, UK to demonstrate its performance. Our results show considerable saving opportunities for customers compared to past studies, which focused on tariff switching alone. The best recommendation model achieves a mean accuracy of 77% and thus largely improves the accuracy of recommendations compared to a designed naive benchmark. Most interestingly, we find that the recommendations can be further improved if customers provide short time series of their historical load data. This encourages retailers and consumers to collaborate in finding the best service bundles.

The remainder of this chapter proceeds as follows: In Section 6.2, we provide a structured overview of related research and identify an important lack of bundle recommendation research in the energy context. In Section 6.3, we present the methodology, including the optimization of technology operation under different set-ups, subsequent label generation, and finally, the classification algorithms used for recommending service bundles. In Section 6.4, we introduce the data set used in the case study, including data on electricity consumption, mobility, electricity prices, and weather. In Section 6.5, we present the case study results. In Section 6.6, we discuss these results, methodical limitations, and potential extensions to our work. Finally, in Section 6.7, we summarize the main scientific conclusions and practical implications for electricity retail managers.

6.2 Related Work

Service bundling describes a marketing strategy in which companies offer a combination of services in one set. Bundling is used in various industries, including communication service providers, e-commerce websites, online movie and music streaming businesses, and video game distribution platforms (Bai et al., 2019; Li et al., 2020). Compared to single item sale, bundling can lead to increased transaction volume and benefit both customers and sellers (Bai et al., 2019). Nevertheless, the majority of recommender research focuses on recommending single products or services, not bundles thereof (Li et al., 2020; Chen et al., 2019). This is also true for recommendation research regarding electricity retail markets. Therefore, we structure this section into two subsections. In the first subsection, we review existing bundle recommendation research in different sectors. In the second subsection, we zoom in on the energy sector, where studies have focused on electricity tariff switching and, so far, neglected bundle recommendations.

6.2.1 Service Bundle Recommendation

Classical bundle recommendation uses customers' historical purchase data and external data to predict their preference for a bundle of items.

Deng et al. (2014) present a recommendation model for a consumer goods shopping website. Their model is based on an extended random walk that uses the social network structure of the website to incorporate the degree of trust between different users. They find that this approach outperforms existing benchmarks in quality and speed.

Pathak et al. (2017) address personalized bundle generation and recommendation on video game distribution platforms. For that, they utilize both data on single item purchases and data on bundle purchases and combine traditional matrix factorization techniques with bundle-specific aspects such as bundle size and item compatibility. This enables them to make robust recommendations via Bayesian Personalized Ranking even for bundles that contain items, which are not contained in any of the training set bundles.

Similarly, Chen et al. (2019) address the issue of limited number of user-bundle transactions. They present a model for collaborative bundle recommendation based on Deep Attention Networks. They apply their model to two case studies: music and books. The authors find that their model outperforms benchmarks and performs best when a) single item embeddings are aggregated in order to obtain a bundle's representation and b) multi-task learning is conducted by integrating user-bundle interactions and user-item interactions with the goal to overcome the limited number of user-bundle interactions.

Bai et al. (2019) cover the case of an online retailer that needs to create bundles from a wide range of different consumer products in order to then recommend a personalized list of diverse bundles. The authors present a neural network based approach for generating and then recommending bundles. Testing their model on public and industrial data sets, they find that their approach improves precision while creating highest diversity among recommended bundles, an aspect that can further increase total transactions.

Ettl et al. (2020) assess data-driven recommendation models for online retail shopping and airline travel booking that include personalized bundle pricing and take into account the sellers inventory. They find that their models increase revenues by 2%–7% compared to current industry pricing strategies and their best model achieves 92% of the revenues of a full-knowledge perfect foresight strategy. Moreover, they find that the largest revenue increase comes from customers with lower price sensitivities, and that the increase in sales volume depends on the product category.

Li et al. (2020) present a literature review of personalized bundle recommendation. They emphasize the increasing importance of bundle recommendation in many people's lives. Besides, they highlight that compared to single item recommendation, bundle sparsity and cold start issues are specific challenges, since customers usually only interact with a small number of bundles, which makes it more difficult to train a well-performing recommendation model.

In summary, multiple studies on service bundle recommendation exist, usually addressing digital products and services. No study in the energy domain can be identified. State of the art methods often rely on Machine Learning approaches. Several studies highlight the cold-start problem of bundle recommendation, which describes that customers with few or no past transactions cannot receive good recommendations (Deng et al., 2014). This problem is common in markets with low purchasing frequency (Backhaus et al., 2010) and thus applies to energy service bundles.

6.2.2 Energy Service Recommendation

Compared to the markets addressed in past studies, the market for energy services has several specific challenges, like a much smaller set of products that can be combined, lower purchasing frequency, and relatively high transaction volume per purchase. These might be the reasons why so far, no study has examined service bundle recommendation in the context of electricity retailing. Instead, studies of energy service recommendation research have focused on the question whether customers should keep their electricity tariff, or switch. Therefore, we briefly review these studies in the following paragraphs.

Ericson (2011) investigates the self-selection of consumers into a CPP tariff. The results indicate that the selection of the CPP tariff depends more on a customer's demand response (i.e. their ability to change their electricity consumption behavior in accordance to the tariff) than on their original consumption patterns. This showcases the need to consider customers' demand response when recommending tariffs.

Arora and Taylor (2016) estimate probability densities for residential electricity consumption and use it to derive electricity cost estimates under different time-varying tariffs. Their approach enables cost savings for the majority of 1,000 customers in a data set from Ireland. Albeit, the magnitude of savings is limited, with around two Euros per customer over a four week period. The study also neglects demand response by customers.

Ramchurn et al. (2013) and Fischer et al. (2013) present an agent based platform for electricity tariff selection. They use historical electricity consumption data from individual households to forecast their hourly consumption, which can then be used for making tariff switching recommendations. For forecasting, Ramchurn et al. (2013) use a Gaussian process approach, which slightly outperforms a naive benchmark that forecasts the mean energy usage from the training data as future values for the test data. In addition, the authors perform load disaggregation for a dishwasher and provide load shifting recommendations for this appliance. However, they quantify neither the financial effects of tariff recommendation, nor of demand response.

Fischer et al. (2013) use a sample of ten households and find that potential yearly savings of £35 - £391 can be achieved by customers if they switch their tariff optimally. User interviews show important barriers for tariff recommendation. First, consumers note that the potential savings they could achieve by following the tariff recommendation system's advice are not high enough for them compared to the effort of switching. Customers said £40-60 per year were too low, but £300 were high enough for considering switching. Second, manual shifting is perceived as a large disutility and not worth the effort. Both these points call for an approach that includes automated control of energy-intensive technologies. Moreover, the accuracy of the recommendations is a big concern (Fischer et al., 2013). This is particularly important, since many residential electricity customers are loss-averse (Nicolson et al., 2017a), which significantly decreases their willingness to adopt time-varying tariffs (Nicolson et al., 2017a).

To shed more light on the topic, Chapter 5 already analyzed the statistical and financial effects of switching to time-varying tariffs. The applied approach recommends the cheapest tariff on the grounds of one month of consumption data. The results show that the reliability of the classifier differs strongly between tariffs, e.g. achieving few false negatives in the case of the Flat tariff and the RTP tariff. The cost associated with picking a non-optimal tariff are especially high for the RTP tariff. In addition, Chapter 5 concludes that more similar tariffs (e.g. different three level TOU tariffs) are more likely to be confused by the recommender, but the costs of confusing such similar tariffs are relatively low. This calls for more sophisticated tariff recommendation methods, e.g. based on Machine Learning.

Luo et al. (2019), Li et al. (2019), and Zhang et al. (2019) propose tariff recommender methods for residential customers based on collaborative filtering, using key electricity consumption features of customers. Evaluating their models across different data sets, the studies find that collaborative filtering outperforms naive (Luo et al., 2019; Zhang et al., 2019) and cluster based (Zhang et al., 2019) benchmarks. The studies do not consider energy intensive low-carbon technologies and note this as an important direction of future research (Zhang et al., 2019). An important reason for this is, as noted by earlier studies, the low savings potential of residential customers without energy intensive technologies (Zhang et al., 2019).

In summary, past energy service recommendation research has focused on recommendations for tariff switching. Studies have shown that savings are often too low to motivate consumers to switch, if no demand response, or only manual demand response is considered. This strongly motivates to expand the existing scope of tariff recommendation to bundles of tariffs and sustainable energy technologies like solar PV, batteries, heat pumps, and BEVs, and to include demand response from those technologies. This notion is further supported by the finding that the ability to perform automated demand response has a positive effect on the willingness to adopt time-varying tariffs (Nicolson et al., 2018). In the case of BEVs, this effect has been shown to be strongest right after the BEV purchase, which further motivates a joint recommendation of technology and tariff (Nicolson et al., 2017b). Besides, the accuracy of recommendations is important, since customers are risk-averse and fear negative consequences of their choices (Nicolson et al., 2017b).

6.2.3 Research Gap

In summary, the review of related work uncovers a key gap in the existing body of research. Previous research has not analyzed bundle recommendations in the energy sector. Multiple studies have focused on tariff recommendation and found that savings from tariff switching alone are too low to motivate consumers to switch. Households with energy-intensive technologies however, show higher willingness to switch tariffs. Thus, it is promising to include energy-intensive technologies and their automated demand response in the recommendation step, i.e. develop a recommendation tool for sustainable energy services bundles.

Compared to traditional tariff-only recommendation approaches, this poses several novel challenges. The additional volatility and unique characteristics of PV, HPs, and BEVs need to be captured by novel data analytics solutions (vom Scheidt et al., 2020, 2021). Corresponding models thus face considerable additional complexity compared to a tariff-only recommendation model and thus should be tackled with state-of-the-art Machine Learning models.

Furthermore, the adoption of such bundles might have much larger economic impacts for residential customers than tariff switching alone. Higher savings could improve the cost/benefit ratio of switching tariffs. Therefore, it is important to quantify the economic consequences of these recommendations.

Even more importantly, no study to date has assessed the role of input data on the quality of recommendations. It is therefore interesting to differentiate between easy-to-obtain data, like the direction of the customer's roof, and more sensitive customer data recorded by smart meters. This way, it can be identified if customers can benefit from sharing their smart meter data with the retail company and in turn receive improved recommendations that are more reliable and enable higher savings for them.

To address these gaps, we next present and evaluate the first data-driven decision support tool for recommendations of energy service bundles, incorporating customers' consumption data. The approach assumes that all bundles deliver the same value to each customer, i.e. meeting their needs for electricity, heating and mobility, but come at different costs. Our goal is to identify and then recommend the bundle with the lowest annual costs for each individual customer, based on household and consumption characteristics. This approach is described in detail in the following section.

6.3 Methodology

In this section, the chapter's applied methodology is presented which is aimed at recommending cost minimal energy service bundles is presented. A bundle consists of a heating technology, a mobility technology, an electricity tariff, as well as optionally a solar PV plant and a battery storage. Importantly, the usage period of the recommended service bundle is one year: All technologies are leased for the duration of one year and the contract period of the tariff is also one year. Figure 6.1 shows the overall methodology. First, the sample set is generated. Second, the operation of various technology and tariff combinations in a household's home energy management system is optimized. Third, the resulting optimal operation costs and additional capital costs are used to generate the class labels for all samples. The class samples are the optimal service-tariff bundles for each household. Fourth, we develop and evaluate Machine Learning models that recommend optimal tariff-service bundles, i.e. derive the optimal class of each sample a priori, only using easy-to-obtain customer data and, in an alternative scenario, additional sparse historical consumption data.

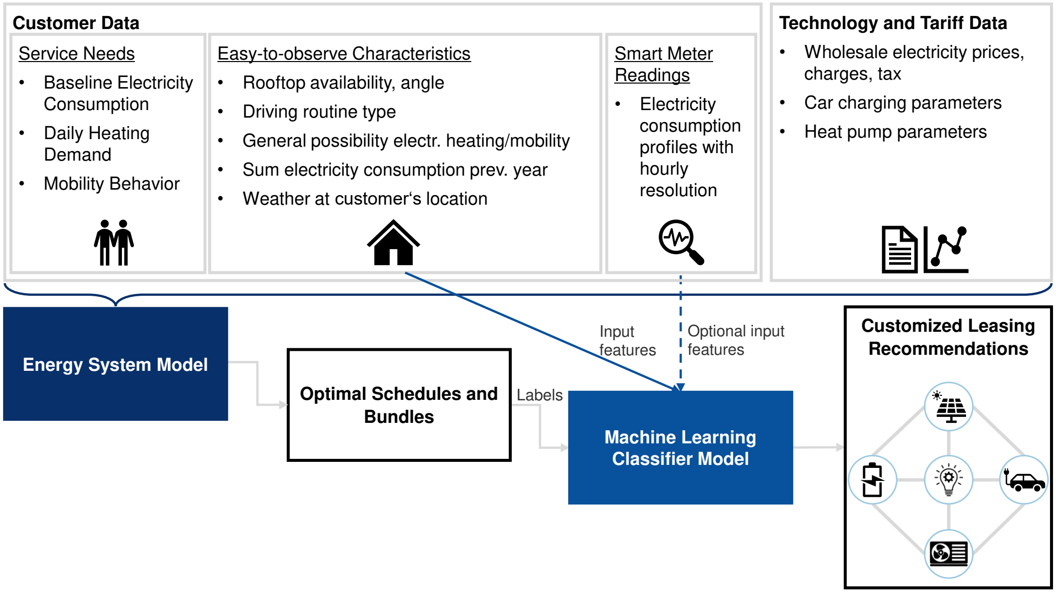


Figure 6.1.: Method overview

6.3.1 Sample Set Generation

Many traditional recommender systems rely on large data sets from frequent customer transactions (Li et al., 2020) and try to identify a bundle that delivers maximum value to a customer. Due to the cold-start problem (compare Section 6.2), traditional approaches are inadequate for our use case. Instead, innovative approaches are needed to create a labelled data set. Therefore, we conduct a dedicated smart home energy management optimization to create samples and labels.

This study is carried out on the basis of data from individual households. Each household is characterized by an empirical electricity load profile that comprises its base electricity consumption over two years at an hourly resolution, and an empirical driving profile that captures the exact driving behaviour over one week. In addition, each household is characterized by individual circumstances that influence if it can adopt a certain energy technology.

The most important distributed energy technologies include rooftop solar PV for the on-site generation of sustainable electricity, electric heating and electric vehicles for the direct use of electricity for domestic heating and mobility needs, and home batteries for the local storage of electricity (see International Energy Agency (2021b)). These technologies are therefore considered in the case study. The relevant household parameters thus include the general binary technical feasibility of an electric vehicle or electric heating in a household. For example, it could be infeasible for customers to adopt an EV because they live in an apartment and have no charging option. Besides these two parameters, households are characterized by the binary availability and azimuth (East, South, or West) of the house's rooftop, and the driving routine type (existence of a commuter in the household or not). Table 6.1 summarizes these external parameters. By combining all given load profiles with all potential external parameter combinations, we expand and diversify the original data set and the number of samples, which enables us to derive more insights about the determining factors of optimal tariff-service bundles.

Table 6.1.: Morphological box of externally given circumstances

Parameter	**Values**			
Azimuth	No solar possible	90	180	270
Driving routine	Non-commuter	Commuter		
Vehicle	EV impossible	EV possible		
Heating	HP impossible	HP possible		

Since the mere feasibility of a certain technology does not automatically mean that its use is cost-optimal for a household, we explore a number of different bundle options for each household under the given external restrictions. Each bundle includes an electricity tariff, a heating technology (heat pump vs. gas heating), a mobility technology (EV vs. combustion engine car), and can include an optional roof-top solar PV system, and an optional home battery storage. The tariff options include the four most common kinds of electricity tariffs in research and practice. These are a standard Flat tariff, a time-of-use tariff with two price levels (TOU-2), a time-of-use tariff with three price levels (TOU-3), and an RTP tariff. While Flat tariffs represent the predominant reference tariff for most residential customers (European Union Agency for the Cooperation of Energy Regulators, 2016), RTP tariffs link consumers' electricity prices directly to wholesale prices and thus incorporate both the risk of increasing, and the chance for reduced bills (vom Scheidt et al., 2019; Burger et al., 2020). Under TOU tariffs, the price levels are determined in advance and repeated at different times of the day, days of the week or seasons and act as a proxy of RTP tariffs. Table 6.2 summarizes these bundle design options.

Table 6.2.: Morphological box of service bundle design options

Service	Design options			
Tariff	Flat	TOU-2	TOU-3	RTP
PV	PV system		No PV system	
Heating	Heat pump		Gas heating	
Mobility	Electric vehicle		Combustion engine vehicle	
Storage	Battery storage		No storage	

6.3.2 Optimization

To determine the costs of operating different tariff-service bundles for a household, we model the technology operating strategy as an optimization problem. The optimization problem minimizes the costs under each of the possible electricity tariffs that result from serving a given electricity consumption profile and the electricity demands of the HP and the EV, if applicable. For this purpose, the optimization makes use of the temporal flexibility of the applied technologies. Our optimization model is executed for all possible combinations of external circumstances and potential technologies. For example, if the external circumstances forbid usage of an EV, only bundles without EVs are considered in the optimization for the given household. For modelling purposes, we assume perfect foresight within one day, as there are various well-performing methods for short-term forecasting of electricity generation, loads and prices (see vom Scheidt et al. (2020) and Chapter 7 and 8), car trips (Huber et al., 2020), and weather (Fathi et al., 2021). Besides, electricity prices for customers are often known in advance if based on day-ahead wholesale prices (like in our RTP tariff) or fixed for longer periods (like in the Flat and TOU tariffs). We furthermore assume no manual adjustment of base consumption (e.g. switching on the dishwasher at a certain time of the day), because transaction costs of behavioral change can render manual demand response non-profitable and empirical programs have found substantially higher electricity demand elasticity for households with automated technology (Schneider and Sunstein, 2017). Capital costs are not considered in the optimization, but are later added for each bundle (see Subsection 6.3.3).

The optimization uses an hourly time resolution and is performed over an entire year, for each year individually. The objective function minimizes the sum of the costs for meeting the electricity demand over all hours within the respective year (see Equation 6.1). Here, $griddemand_h$ is the amount of externally sourced electricity in hour h in kWh. It is multiplied with the price of one kWh of electricity ep_h^{tariff}, which depends on the type of tariff and hour h. The model considers remuneration for the feed-in of PV-generated electricity, where $supply_h$ is the amount of electricity in kWh fed into the grid in hour h, and $ep^{feedin-tariff}$ is the invariable feed-in tariff in £/kWh.[11] This compensation is subtracted from the costs of externally sourced electricity.

$$\min \sum_{h=0}^{8759} griddemand_h \cdot ep_h^{tariff} - gridsupply_h \cdot ep^{feedin-tariff} \tag{6.1}$$

The total hourly electricity demand consist of the inelastic base electricity use c_h^{base}, the electricity consumed by the heat pump c_h^{hp}, the electricity needed for charging the electric vehicle ch_h^{ev} and the battery storage $ch_h^{storage}$, and the part of the solar plant's generation that is fed into the grid $gridsupply_h$. Equation 6.2 guarantees that the total energy demand in every hour h within the one-year period is met by the sum of the purchased electricity $griddemand_h$, the solar PV based self-generation pv_h and the energy discharged from the battery storage unit $dc_h^{storage}$. It therefore ensures that electricity demand and supply are always balanced. Moreover, the equation ensures that PV based electricity is either directly consumed, fed into the household battery for later use, or fed into the grid at a fixed feed-in remuneration. For all bundles without electric heating or electric mobility, we add the costs of the non-electric alternative, i.e. natural gas for bundles with gas heating, and gasoline for bundles with internal combustion engine vehicles, after the optimization.

$$\begin{aligned} c_h^{base} + c_h^{hp} + ch_h^{ev} + ch_h^{storage} + gridsupply_h \\ \leq pv_h + dch_h^{storage} + griddemand_h, \ \ \forall h \in [0, 8759] \end{aligned} \tag{6.2}$$

In Equations 6.3 to 6.4, the charging state of the EV $state_h^{ev}$ is defined and con-

[11]Note that, because the electricity consumption data set is from London, UK (see Section 6.4.1), we perform all financial calculations in British Pounds.

strained. $evbi_{h-1}$ is a binary parameter and determines if charging of the battery is possible in hour $h-1$. This is the case, if the EV is parked at home throughout the entire hour. For each hour in which the EV leaves for a trip, the required energy for that trip is specified via dch_h^{ev}. In hours in which the EV does not leave for a trip, the required energy dch_h^{ev} is zero.

$$state_h^{ev} = state_{h-1}^{ev} - dch_{h-1}^{ev} + evbi_{h-1} \cdot ch_{h-1}^{ev}, \ \ \forall h \in [1, 8759] \tag{6.3}$$

As it is assumed that the BEV is only charged at home, $state_0^{ev}$ always needs to be sufficiently high to provide the energy for the entire following trip (Equation 6.4).

$$state_h^{ev} \geq dch_h^{ev}, \ \ \forall h \in [0, 8759] \tag{6.4}$$

At time $h = 0$, the charging level of the car's battery starts at $state_0^{ev} = 0$ (Equation 6.5).

$$state_0^{ev} = 0 \tag{6.5}$$

The battery storage's behaviour is similarly described in Equations 6.6 to 6.9. $state_h^{storage}$ is the battery storage's state of charge at hour h and depends on the charge and discharge amounts $ch_{h-1}^{storage}$ and $dch_{h-1}^{storage}$ in the previous time period $h-1$ and the previous state of charge. In the first hour, the initial charging state $state_0^{storage}$ of the battery storage is zero. Simultaneous charging and discharging of the battery is forbidden.

$$state_h^{storage} = state_{h-1}^{storage} + ch_{h-1}^{storage} - dch_{h-1}^{storage}, \ \ \forall h \in [1, 8759] \tag{6.6}$$

$$state_0^{storage} = 0 \tag{6.7}$$

$$dch_h^{storage} \leq state_h^{storage}, \ \ \forall h \in [0, 8759] \tag{6.8}$$

$$ch_h^{storage} \cdot dch_h^{storage} = 0, \ \ \forall h \in [0, 8759] \tag{6.9}$$

The use of the heat pump is defined by Equations 6.10 to 6.14. Equation 6.10 ensures that the heating demand of each day (hd_k) is always met. The heat production in every hour of the corresponding day is hp_h. It depends primarily on the outdoor temperature, which is reflected in the coefficient of performance COP_h, as the efficiency of air heat pumps is lower at lower outside temperatures (Equation 6.13). For reasons of simplification, we assume that the heat pump runs on full capacity, when active. Heat generation therefore always generates a power consumption equal to the heat pump's maximum capacity hp_cap for every heating hour (Equation 6.12). Whether heating takes place in hour h is described by the binary variable $heatbi_h$. Losses in the switch-on and switch-off processes are generally not taken into account. To reduce the potential impact of this limitation, Equation 6.11 ensures that heating is always performed consecutively within a day. In other words, the heat pump is only activated once a day. $nheat_h$ specifies how many hours of heating are necessary with a start in hour h to fulfill the daily heat demand hd_k. Heating storage is implicitly considered and is assumed to be operated such that the produced heat energy is distributed over the corresponding day.

$$\sum_{h=24k}^{24k+23} heatprod_h \geq hd_k, \ \ \forall k \in [0, 364] \tag{6.10}$$

$$\sum_{x=h}^{h+nheat_h} heatbi_x \geq nheat_h \cdot (heatbi_h - heatbi_{h-1}), \ \ \forall h \in [1, 8752] \tag{6.11}$$

$$c_h^{hp} = heatbi_h \cdot hp\_capa, \ \ \forall h \in [0, 8759] \tag{6.12}$$

$$heatprod_h = COP_h \cdot c_h^{hp}, \ \ \forall h \in [0, 8759] \tag{6.13}$$

$$hp_0 = 0 \tag{6.14}$$

The grid feed-in cannot be larger than the electricity generated by the solar PV system (Equation 6.15). Technical data and constraints of the electric vehicle and battery storage are incorporated through Equations 6.16 to 6.19.

$$gridsupply_h \leq pv_h, \ \ \forall h \in [0, 8759] \tag{6.15}$$

$$state_h^{ev} \leq state_{max}^{ev}, \ \ \forall h \in [0, 8759] \tag{6.16}$$

$$ch_h^{ev} \leq ch_{max}^{ev}, \ \ \forall h \in [0, 8759] \tag{6.17}$$

$$state_h^{storage} \leq state_{max}^{storage}, \ \ \forall h \in [0, 8759] \tag{6.18}$$

$$ch_h^{storage} \leq ch_{max}^{storage}, \ \ \forall h \in [0, 8759] \tag{6.19}$$

Finally, the mathematical domain of all variables is set in Equations 6.20 - 6.23.

$$\begin{aligned} &pv_h, state_h^{ev}, state_h^{storage}, griddemand_h, gridsupply_h, c_h, ch_h^{ev}, \\ &ch_h^{storage}, ch_h^{hp}, dch_h^{ev}, dch_h^{storage}, heatprod_h \geq 0, \ \ \forall h \in [0, 8759] \end{aligned} \tag{6.20}$$

$$evbi_h, heatbi_h, \in \{0, 1\} \ \ \forall h \in [0, 8759] \tag{6.21}$$

$$hd_k \geq 0, \ \ \forall k \in [0, 364] \tag{6.22}$$

$$nheat_h \in \mathbb{N}, \ \ \forall h \in [0, 8752] \tag{6.23}$$

6.3.3 Label Generation

Within the optimization, only the operating costs are considered. To arrive at the final total cost for each bundle, two additional steps are needed. First, capital costs for the used technologies are incorporated (see Subsection 6.4.3). Second, for bundles that include non-electric alternative technologies, fuel costs need are added to allow full comparability. If an electric vehicle or a heat pump are not included in a bundle in the optimization, costs for natural gas and gasoline have to be added to the extent that the same heat load and driving mileage can be covered. This makes the bundles fully comparable in regards to their costs. Based on this cost comparison, the households' cost-minimal tariff-service bundles are derived. Each household's lowest-cost bundle then represents that household's label for the subsequent classification.

6.3.4 Service Bundle Recommendation

The derived labels serve as output vector of the recommendation models. Based on specific input features, the models aim to recommend the cost-minimal bundle. Here, the recommendation of technologies means that they should be leased for the following year, and the recommendation of a tariff means that it should be contracted for the following year.

We develop two models, namely an XGBoost model (XGB) and a feed-forward artificial neural network model (ANN). We assess the models regarding statistical performance, by calculating their accuracy and regarding economic performance, by calculating mean annual costs for customers. Along these two metrics, the models are compared to the theoretical optimal result and to a naive benchmark that simply recommends the most frequent optimal service bundle.

XGBoost is a gradient boosting based ensemble technique that has performed well in many Machine Learning challenges and delivers very good results on different problem types, including on imbalanced data sets like in our case as shown in Subsection 6.5.1 (Nielsen, 2016; Chen and Guestrin, 2016; Hyndman and Athanasopoulos, 2018). A detailed description of the XGB model can be found in Chen and Guestrin (2016). We tune three important hyperparameters via a grid search. The parameters and the tested values are displayed in Table 6.3.

Table 6.3.: Tuned XBG hyperparameters

Hyperparameter	**Values**
Learning rate	0.001, 0.01, 0.1
Minimum child weight	1, 4, 7
Maximum depth	3, 6, 9

ANN models are used in many data analytics applications in the energy context and show good performance in many cases (vom Scheidt et al., 2020). For the ANN in our study, we use an architecture with one hidden layer with a relu activation function, and an output layer with a softmax activation function. We use the Adam optimizer and the categorical crossentropy loss function. Three hyperparameters are tuned using grid search, as shown in Table 6.4.

Table 6.4.: Tuned ANN hyperparameters

Hyperparameter	**Values**
Learning rate	0.001, 0.01, 0.1
Batch size	32, 64, 128
Number of units in dense layers	10, 30, 50

After comparing the performance of the two models, we select the one with better economic performance and use it to compare model performance under different feature subsets (see Subsection 6.4.4). For the comparison, we train models with a) only the easy-to-obtain data, b) easy-to-obtain data and additional weather data, and c) easy-to-obtain data, weather data, and four-week excerpts of smart meter data at an hourly resolution. The goal of that comparison is to identify the value of different data types. Furthermore, we assess four different times of the year for smart meter data collection, i.e. February, May, August and November in order to understand the benefits of data collection during specific times of the year.

6.4 Data

This section describes the data used within this case study in detail.

6.4.1 Electricity Consumption Profiles

The residential electricity consumption data comes from the Low Carbon London project (kaggle, 2019). It includes electricity consumption profiles of 324 households at half-hourly resolution from 2012 to 2013.[12] Since only private households are considered in our case study, we discard 32 outlier load profiles with an unusual low (below 1,000 kWh) or high (above 10,000 kWh) annual consumption in the first year's data set. This results in a final data set of 292 electricity consumption profiles. As described in Subsection 6.3.2, these electricity consumption profiles form the basis for the construction of a total data set of 9,344 households. Figure 6.2 shows the development of the average daily electricity consumption in both years. A clear seasonality can be observed, with higher electricity consumption in the colder seasons. The data patterns are very similar over the two years, with the second year showing an increased level in the first months of the year. The distribution of annual electricity consumption per household is presented in Figure A.1 in Appendix C, also showing great resemblances over both years.

6.4.2 Electricity Tariffs

The electricity tariffs applied within this chapter are designed based on the wholesale electricity prices on the day-ahead market in the UK in 2018 and 2019 (ENTSO-E, 2021). The data sets have an hourly resolution. This subsection provides a short overview of how the electricity tariffs for this analysis are engineered. A more

[12] 2012 was a leap year and thus includes data from February 29th. To achieve better transferability and generalization of the data, the year is treated as if it was not a leap year and the corresponding additional 29.02 data are deleted. The half-hourly data are transformed into hourly values.

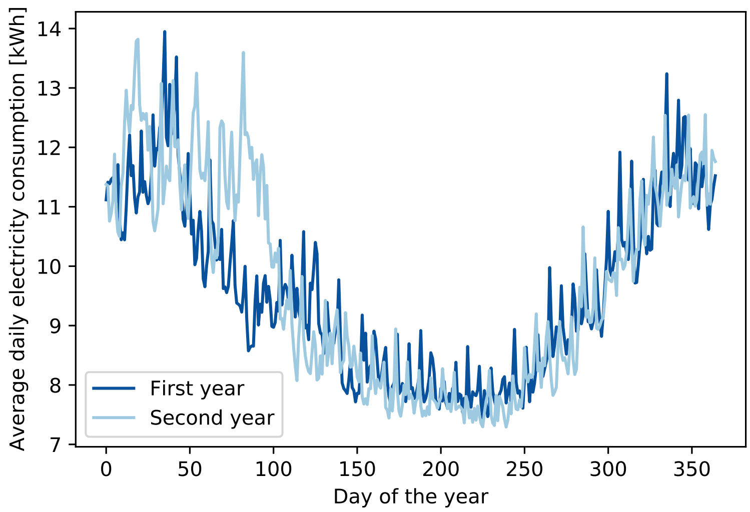


Figure 6.2.: Average daily electricity consumption per household over the course of a year

detailed description can be found in Appendix C.2. Importantly, like in Chapter 5, all tariffs are designed to be revenue neutral ceteris paribus (i.e. before demand response), as full cost recovery is a key principle in tariff design (Bonbright, 1961).

The electricity price in the Flat tariff ep^{flat} is designed by calculating the sum of hourly wholesale prices $wp_{d,h}$ – with d being the day of the year, and h being the hour of the day – weighted by the average hourly electricity consumption of all consumption profiles in the corresponding hour $y_{d,h}$, divided by the total annual consumption. This results in a Flat tariff ep_t^{flat} of 0.059 £/kWh for the first year, and 0.045 £/kWh for the second year.

For TOU-2 and TOU-3, the tariffs are determined as weighted averages of wholesale prices and electricity consumption within the daily recurring time window.

For the TOU-2 tariff, there are two price levels, i.e. “low”, between 11pm - 5 am, and “high”, between 6am - 10pm, with prices of 0.05 £/kWh (0.037 £/kWh in the second year), and 0.062 £/kWh (0.048 £/kWh in the second year), respectively.

For the TOU-3 there are three price levels, i.e. “low” between 11pm - 5 am, “high” from 6am - 3pm and again from 9pm - 10pm, and “peak”, between 4pm - 8pm, with prices of 0.05 £/kWh (0.037 £/kWh in year two), 0.057 £/kWh (0.044 £/kWh), and 0.073 £/kWh (0.056 £/kWh), respectively.

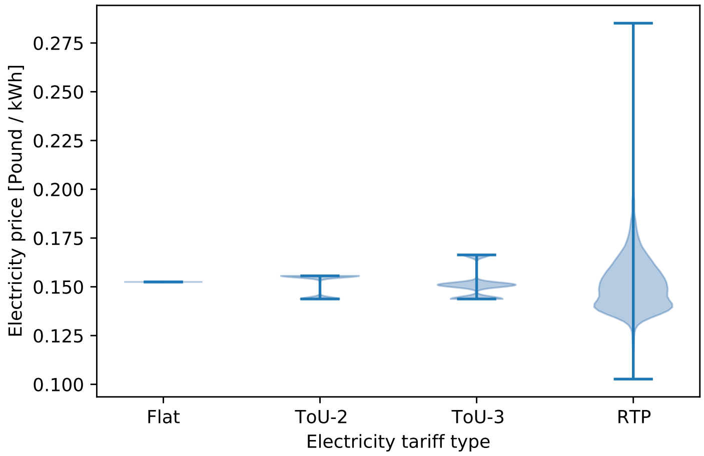


Figure 6.3.: Distribution of variable unit prices over electricity tariffs in the first year

The last tariff to determine is the RTP tariff ep_t^{rtp}. Here, wholesale prices at every hour of the year wp_t are directly passed on to the consumers.

Once these wholesale based electricity prices are determined, grid fees, policy charges and other charges are added in order to receive the final end-user prices. In many geographies, this includes a fixed annual or monthly charge and a volumetric per-kWh charge. Therefore, we add a fixed charge of 94 £ per year, based on the actual charge in London in 2019 (UK National Statistics, 2021a), and a volumetric charge of 0.0936 £ (0.1183 £ in year two), chosen so that the Flat tariff is equal to the average variable unit price in the UK in 2018 and 2019, respectively (UK National Statistics, 2021a). Figures 6.3 and 6.4 display the distribution of the final electricity unit prices for each tariff type in the first and second year, respectively.

6.4.3 Technology Data

In this subsection, the techno-economic data regarding the different energy technologies are described.

Photovoltaics

The data on electricity generation from PV systems is simulated based on Renewables.ninja (2021), using historical data on PV electricity generation in London in

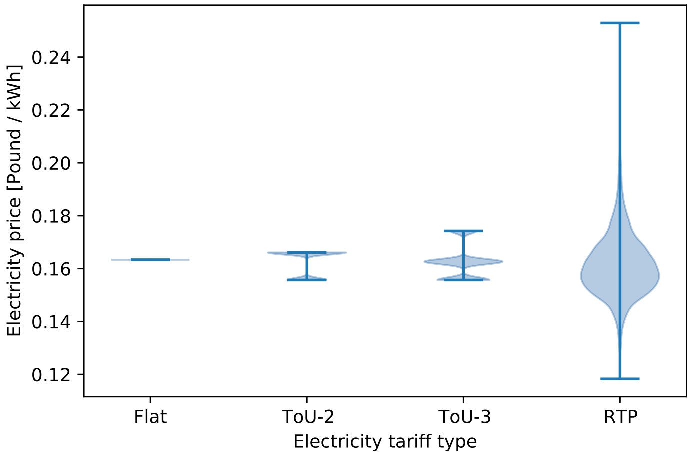


Figure 6.4.: Distribution of variable unit prices over electricity tariffs in the second year

2012 and 2013 with an hourly resolution. A standard tilt of 25 degrees is assumed and a standard system size of 7.48 kWp is chosen, based on the average PV capacity per system installed in Great Britain in 2020 (pv Europe, 2020).
The azimuth is varied according to Table 6.1, resulting in three different electricity generation profiles.[13]

Battery storage

The size of the battery storage is adjusted to the average electricity consumption of the households considered here, which lies under 4,000 kWh. Following the approach by Henni et al. (2021), this results in an assumed battery capacity $state_{max}^{storage}$ of 6 kWh. Its charging takes place at the standard charging power in the UK grid of $ch_{max}^{storage} = 3$ kWh.

Heating

For serving the customers' needs for space heating and warm water, we consider an electric air-to-water heat pump with a standard power PHP of 9 kW (Kümpel, 2021).
The total heating demand of households can be estimated based on the households'

[13]Following the procedure for the electricity consumption data, the data for February 29th 2012 is deleted.

annual electricity consumption in the first year and can be distributed over the year based on outdoor temperature.

Thus, on heating days (i.e., days with a daily average temperature of under 12°C (Recknagel et al., 2006)), the heat pump has to meet space heat and hot water demand, whereas on non-heating days it only has to meet hot water demand.[14]

Mobility

For meeting the customers' mobility needs, we consider an EV with current technical data, i.e. a battery capacity $state^{ev}_{max}$ of 50 kWh, a maximum charging power of 11 kWh ch^{ev}_{max}, and an electricity consumption of 20 kWh per 100 km (International Energy Agency, 2018).

In order to simulate the electricity demand of an electric vehicle, it is necessary to take mobility profiles of the households into account, which include the distances traveled, times, and durations of trips by car. Since the respective mobility information of the households is not available, it is constructed based on empirical data from Ecke et al. (2019). In order to differentiate between different driving patterns, we use a commuter and a non-commuter driving profile for each power consumption profile (see Table 6.1).[15]

Capital Cost

For generating the final labels, capital costs of the technologies need to be added to the operational costs before determining the cost-minimal bundles.

In cases where a time-varying electricity tariff (TOU or RTP) is applied, the use of a smart meter is necessary. For this technology, residential customers are assumed to pay a typical annual fee of 51 £ per year in line with Gausden (2021).

For a 7-8 kW PV system, the average capital costs in 2020 were 9,071 £ (Märtel, 2021).[16] These costs are discounted over the assumed lifetime of twenty years (German Ministry of Finance, 2000), assuming a weighted average cost of capital (WACC) of 4%.

Similarly, the capital costs for the 6 kWh sized storage are estimated to be 2,400 £,

[14]More details can be found in Appendix C.3.
[15]More details can be found in Appendix C.4.
[16]using a EUR:GBP conversion rate of 1:0.854.

following IRENA International Renewable Energy Agency (2017). These costs are annualized based on a life time of ten years and a WACC of 4%.
Unlike PV and battery, the heat pump is a substitute for an existing technology, in most cases conventional gas heating. Since similar costs can be assumed for both kinds of technologies, no additional acquisition costs for the heat pump are assumed. Similarly, it can be assumed that an electric vehicle is a substitute for a conventional vehicle. Since the capital costs of an electric vehicle are often still higher than those of a combustion engine car, we include additional capital costs of 4,000 £, based on Yurday (2020, 2021). Moreover, since this case study assumes charging of the EV at home, the installation of a wallbox is necessary. This results in additional costs of 1,400 £ (500 £ material costs and 900 £ installation costs), based on Autokostencheck (2021); Wallbox.com (2021). The total additional capital costs of 5,400 £ are discounted over ten years with a WACC of 4% and the discounted annual rates are added to the optimization results, correspondingly.

Reference Technology Operation Costs

To enable a fair comparison, the operation costs of alternative, non-electrical technologies for heating and mobility need to be included at a level that meets the same needs for heating and driving.
The heating costs of a gas heater can be calculated based on the average natural gas prices in London in 2018 and 2019 mapped to the two considered years (UK National Statistics, 2021b). Similarly to the electricity cost, they consist of a fixed yearly price and a variable unit price. This leads to yearly fixed costs of 92.51 £ for each household supplemented by operating costs of 0.0389 £/kWh in the first year and fixed costs of 99.29 £ with a unit price of 0.0394 £/kWh in the second year. The costs of operating an internal combustion engine vehicle are based on the average London gasoline prices of 2020 of 1.14 £/liter (UK National Statistics, 2021c) and an average consumption of 7.8 liters per 100 km (Kords, 2020).

6.4.4 Machine Learning Input Data

The Machine Learning models are trained based on various input data, i.e. features that can be categorized into three groups.

The first group consists of **easy-to-obtain data**. This includes the households' external parameters, which are one-hot encoded, i.e. azimuth of roof, driving routine, and feasibility of BEV and HP, as defined in Table 6.1.

The second group contains **weather data** from London (kaggle, 2019). We use temperature, visibility and wind speed data at an hourly resolution. For each of the three, we calculate the monthly mean, standard deviation, maximum, and median value.

The third group consists of **collaborative data** that customers can choose to make accessible to the retailer in order to enable them to make better recommendations. These data comprise hourly smart meter readings. To utilize those time-series data, we engineer the following features: the mean, standard deviation, maximum, and median consumption of the total time series. Additionally, the mean, maximum and standard deviation for the hour-to-hour difference are calculated and included in the feature set. Lastly, the mean for each hour of the day is aggregated to capture daily patterns.

For the Machine Learning task, the data set is split into training, validation and test sets. This split is done in two dimensions, i.e. by year and customers. All training and validation takes place on data of the first year. The subsequent evaluation takes place on data of the second year. We control that all household samples with the same underlying inelastic electricity consumption profile are assigned to only one of the three data sets (training, validation, or test) to prevent the models from learning patterns between customers that are based on the same consumption profile. Under this limitation, 70% of customers are randomly assigned to the training set, 15% are assigned to the validation set, and 15% are assigned to the test set. We repeat the process of data splitting, model training, and evaluation three times, to cross-validate our results.

The models are executed on a Windows computer with Intel i7 core, 1.80 GHz and 16 GB RAM. The computation time for training, validating and testing the XGB model is on average 164 seconds. In comparison, the average computation time for the ANN model is 169 seconds.

6.5 Results

In this section, the results of the optimization and of the recommendation tool are presented.

6.5.1 Smart Home Energy Management Results - Label Distribution

In this subsection, we evaluate the distribution of the resulting cost minimal tariff-service bundles amongst customers.

Bundle frequency

The combination of the four potential technology options with the four tariffs means that 64 bundle labels are generally possible. However, most of these bundles are never optimal and thus do not occur as label. Within the first year's optimal solution, 17 different service bundles appear (23 in the second year). The most common bundle is a Flat tariff in combination with no technology, with 3,932 cases (42.08%) in the first year and 4,433 cases (47.44%) in the second year. This large share is driven by the fact that we deliberately design and include customer samples for whom it is externally impossible to use a PV plant, a BEV, and a heat pump (see Subsection 6.3.1). The second most common bundle with 1,710 (18.30%) cases (1,751 or 18.74% in year 2) features the use of an RTP tariff in combination with an electric vehicle. The third most frequent bundle constitutes the application of a heat pump under the RTP tariff with 1,513 customers (16.19%) in year 1 and 516 customers (5.52%) in year 2. An overview of these and all further bundles and their occurrences can be found in Table 6.5. A “1” in the respective technology's column means that that technology is part of the optimal bundle, whereas a “0” means that it is not.

Individual Technology and Tariff frequency

Regarding the different technologies, the installation of a PV plant, independent of its azimuth, is part of the most profitable service bundle in 18.8% (27.8% in the second year) of the possible cases. Of these cases, about half include a south-facing PV system, and about a quarter each includes east and west facing orientation,

Table 6.5.: Frequency of bundle occurrence in both years' data

Bundle (Label)					**Frequency**	
PV	HP	Storage	BEV	Tariff	Year 1	Year 2
0	0	0	0	Flat	3,932	4,433
0	0	0	1	RTP	1,710	1,751
0	1	0	0	RTP	1,513	516
0	1	0	1	RTP	671	231
1	1	1	1	RTP	551	660
1	1	1	0	RTP	511	755
1	0	1	1	RTP	183	296
0	0	0	1	Flat	52	60
0	0	1	1	RTP	42	151
0	0	0	0	RTP	40	24
0	1	1	0	RTP	36	101
1	0	0	1	RTP	33	78
1	0	1	0	RTP	29	89
0	0	1	0	RTP	15	24
0	1	1	1	RTP	14	48
1	0	0	1	Flat	9	42
1	1	0	1	RTP	3	2
0	0	0	0	TOU-3	0	40
1	0	1	0	Flat	0	14
1	0	0	0	Flat	0	12
0	0	0	0	TOU-2	0	12
0	0	0	1	TOU-3	0	4
1	0	0	1	TOU-2	0	1

respectively. The electric vehicle is part of the optimal bundle in roughly 70% of the cases in which it is externally possible, in both years. The majority of these cases belongs to customers with commuter driving profiles, which indicates that differentiating regarding driving profile types can be relevant for optimal bundle selection. The heat pump's usage is part of the optimal bundle in 70.6% (49.5% in the second year) of the possible cases. The installation of a battery storage is always possible and occurs in 14.8% (22.9%) of the cases. In the vast majority of these cases, the battery is combined with a PV system, which hints at the saving potentials from self-consumption. Nevertheless, in 7.75% (15.15%) of the cases in which a battery is used, it is used without a PV system, but with the RTP tariff. In these cases, the advantage of the battery storage results solely from charging it with grid electricity in low-price hours that is later supplied to the customer behind the meter.

The standard Flat tariff finds application in 42.6% (48.8%) of the most profitable service bundles. 57.4% (50.6%), and thus the majority of cases, contain the RTP-tariff. This shows the high potential of this electricity tariff. While in most cases, the combined usage of technologies renders the RTP tariff beneficial, in a few cases (0.43% in year 1 and 0.26% in year 2), the customer's electricity consumption profile alone allows the household to benefit from the RTP tariff even without additional technologies. Besides, it becomes evident that the TOU tariffs are not attractive in this model setting. TOU-2 and TOU-3 are not part of any cost-optimal bundle in the first year. In the second year, all tariffs occur, but TOU tariffs only occur in 0.61% of the optimal bundles.[17]

Effects of bundling on technology selection

To isolate the effect of combining electricity tariffs and technologies in bundles on optimal recommendation, we compare these results to a scenario in which the given Flat tariff is the only possible tariff option. This artificial limitation leads to results that differ in varying degrees from the tariff-service bundle recommendations. In the absence of time-varying tariffs, PV systems are chosen in 23.8% (36.6%) of the cases, constituting a small, but considerable increase. Batteries find application in 11.2% (11.8%) of the most profitable service bundles, constituting a small decrease. Notably, the use of batteries now takes place exclusively in combination with an installed PV system, since the absence of time-varying prices prohibits other applications than maximization of self-consumption. The absence of time-varying prices furthermore decreases the occurrence of BEVs in the optimal bundle from roughly 70% to 65% in both years, and the occurrence of heat pumps (which have even more flexibility) to 32.5% (22.0% in the second year) from 70.6% (49.5%) of cases, which constitutes a reduction of more than 50%. In summary, these comparisons demonstrate the synergies between innovative tariffs and distributed energy technologies and strongly motivate their bundled recommendation.

[17] In practice, additional factors such as transaction costs, simplicity, and acceptance might increase the attractiveness of TOU tariffs, compared to RTP.

Label distribution

The retrieved optimal bundle for each household is also the label for the subsequent Machine Learning classification task. The distribution of labels is imbalanced, because some labels occur much more frequently than others. In particular, it can be a challenge to adequately recommend bundles that only occur very rarely or not at all in the training set of year 1.

6.5.2 Service Bundle Recommendation

This subsection presents the results of the different recommendation methods. In the first paragraph, the three described Machine Learning methods are compared. In the second paragraph, three models based on different feature subsets are compared.

The accuracy is evaluated as it is the most intuitive measure to understand the classifiers performance. As the underlying data set is imbalanced, the accuracy must be evaluated in comparison to the baseline model. Besides accuracy, the mean economic performance is evaluated as it is the natural target metric of the economic case presented and therefore the given recommendation shows the actual performance of a method on that task.

Comparison of methods

First, we compare the performance of the two Machine Learning methods, the naive benchmark, and the optimum. The calculated mean energy costs (economic evaluation) and the classification accuracies are given in Table 6.6. The table shows that the XGB model and the ANN model outperform the dummy classifier regarding classification accuracy. The ANN model achieves 77% accuracy, the XGB model 73%, and the naive benchmark 56%. Besides, both Machine Learning models achieve cost reductions, compared to the naive benchmark. The ANN model achieves mean annual energy costs reductions of 323 £, while the XGB model even results in savings of 334 £. Economically, the models perform close to the theoretic optimum, with a delta of 16 £ (XGB), and 27 £ (ANN) compared to the optimal bundles. This represents a very good economic performance, even if accuracies are not close to 100%. A potential reason for this is that the costs of some sub-optimal bundles are close to those of the optimal bundle. The fact that the ANN achieves slightly better accuracy, but slightly worse cost results indicates that accuracy is not a perfect proxy for economic performance. This motivates a further investigation with methods that utilize the cost associated to the bundles during the training process, i.e. *Learn to Rank* approaches.

Table 6.6.: Accuracy and mean energy costs for different methods

Method	**Mean energy cost**	**Classification accuracy**
Naive	2,972 £	56%
ANN	2,649 £	77%
XGB	2,639 £	73%
Optimum	2,622 £	100%

Comparison of feature subsets

Second, we compare the performance of using different feature subsets. As described in Subsection 6.4.4, there is a different level of difficulty in obtaining different features. Therefore, the performance with and without harder to obtain data is crucial to understanding their value. Table 6.7 shows the performance of the XGB model based on the easy-to-obtain (basic) features, the weather features and the smart meter consumption features. While the XGB model achieves an accuracy of 73% when using all features, it achieves only 59% without the smart meter data. Given that the naive classifier achieves an accuracy of 56%, the results show that most of the correct classifications beyond the majority class are made possible by smart meter consumption data. The mean costs with and without harder to obtain features differ by 20 £. This shows that smart meter data provides additional value, whereas the weather data alone does not. It also indicates that, while the smart meter data are often necessary to find the actual optimal bundle, the easy-to-obtain data are enough to prevent the model from making very cost inefficient predictions.

6.6 Discussion

In this section, limitations of the research presented in this chapter are described, proposals for future work are given and practical implications are discussed.

Table 6.7.: Accuracy and mean energy costs of the XGB model with different input feature sets

Features	Mean energy cost	Classification accuracy
Basic	2,659 £	59%
Basic + weather	2,659 £	59%
Basic + weather + smart meter	2,639 £	73%

This chapter is based on a data set that is subject to several limitations. All households are assumed to make use of a private car and the driving profiles are randomly assigned to the households. It is recommended to collect and use actual household specific data regarding power consumption, mobility behaviour and heating demand in future work. For all technologies, assumptions and simplifications are made that might in some cases not be directly transferable to reality. Among others, the individual empirical heat consumption behavior of households is not taken into account when calculating heating requirements. Instead, average values are used. Different insulation and heat losses of the households are also not taken into account. Additionally, the technology costs assumed here are based on current state-of-the-art data and might vary in the future and be different in other geographies. Future work could expand our approach by including customized sizing of technologies based on household characteristics like number of inhabitants, house insulation, etc. Sensitivity analyses are recommended to be conducted in future work varying technology costs and their WACC.

The optimization is also subject to limitations. It only takes demand response into account for the electricity consumption of newly installed technology. In addition, we focus on costs as the only metric for identifying optimal tariff-service bundles and for making recommendations. Therefore, transaction costs and behavioral considerations that might influence customers' decisions are ignored (Staudt et al., 2019a).

For both evaluated metrics (accuracy and annual costs), we focus on the mean value. We do this, because in an real-world setting, a service bundle provider might choose to guarantee certain cost savings for their customers and internally average the losses and gains of individual customers. Such a novel business model could address risk-aversion among consumers and further facilitate the uptake of the recommended bundles. This chapter's theoretical findings can be supplemented by empirical experiments regarding acceptance of recommendations made with introduced decision support tools. The detailed design of retailers' business models based on this decision support tool is also subject to future research. The generated labels are presumably highly dependant on the applied regulation. Consequently, changes in regulation or the application to other countries make it necessary to retrain the models. Transferring previously trained models to new settings can overcome these problems (Torrey and Shavlik, 2010).

Our study does not consider manual demand response, as it typically represents a smaller potential than the automated demand response of technologies such as electric vehicles and heat pumps in our study. As Schneider and Sunstein (2017) point out, it can be beneficial to use RTP tariffs for technologies with automated demand response and in parallel TOU tariffs for all manually operated electricity consumption. Such manual demand response could be modelled according to Gottwalt et al. (2011) in future expansions of this study.

Moreover, the chance of increased electricity bills resulting from non-optimal recommendations can limit the practical acceptance of the decision support tool immensely. A guarantee of non-increased costs by applying bill protection can eliminate this issue (Nicolson et al., 2018). This can be part of a robust business model that retailers may build based on the developed decision support tool.

6.7 Conclusions

In this section, we summarize the findings of this study and outline management implications.

Our results demonstrate the large benefits of energy service bundles that combine time-varying electricity tariffs with flexible sustainable technologies. We find considerable saving potentials that by far exceed the savings that customers can achieve from tariff switching alone (compare also Chapter 5). The availability of time-varying electricity tariffs makes energy technologies more financially attractive for many households. In the vast majority of cases, the optimal bundles include not only a change of tariff.

Furthermore, our results show that the developed Machine Learning recommendation models achieve accuracies of 73%-77% and thus outperform the naive benchmark (56%). Similarly, they achieve better economic performance, by reducing mean energy costs to 2,639-2,649 £, compared to 2,972£ under the naive benchmark.

Moreover, we find that using 'collaborative data', i.e. four week excerpts of smart meter data that the customers provide to the retailer, improves the mean accuracy of recommendations from 59% to 73% for the XGB model. It also increases the savings potential, by lowering mean energy costs from 2,659£ to 2,639£. Overall, we see good potential for a collaboration between customers and retailers, where data sharing leads to added value on both sides.

This developed decision support tool can help customers to find a personalized tariff-service bundle that lets them benefit from cost savings. At the same time, this increases the diffusion of sustainable energy technologies, tariffs and smart meters, which can be a strong support for the energy transition. The tool may help electricity retailers in their business model transition, highlighting investments that are beneficial and helping them to profit from the ongoing decentralization of the energy sector. Based on our results, we see great potential for further development and application of Machine Learning based recommendation systems, combining the recommendation of tariffs and services as a bundle.

Besides these key results, this chapter also demonstrated that a crucial ingredient for the integration of technologies at the customer level is the operation of batteries, heat pumps, and BEVs in accordance to tariffs. In order to optimize such operation in advance, appropriate short-term forecasts (i.e. forecasts with a horizon of up to one week) of residential electricity loads and generation are needed. Therefore, state of the art methods of short-term forecasting of residential loads are reviewed in Chapter 7 and a new forecasting model is developed in Chapter 8.

CHAPTER 7

THE STATE OF THE ART OF SHORT-TERM RESIDENTIAL LOAD FORECASTING

This chapter analyzes the state-of-the-art approaches in the forecasting literature, with regard to model performance, complexity and running speed, as well as used data sets, feature selection methods, benchmarks methods, and evaluation metrics. Finally, the findings are distilled and guidelines for the development of forecasting models for smart home energy management systems are derived.

Section 7.2, 7.3, and 7.4 of this chapter comprise parts of the published article: F. vom Scheidt, H. Medinová, N. Ludwig, B. Richter, P. Staudt, C. Weinhardt, *Data analytics in the electricity sector – A quantitative and qualitative literature review*, Energy and AI, Volume 1, 2020.

7.1 Introduction

The rising numbers of prosumers with own volatile solar PV generation, and large, varying electricity consumption from heat pumps and electric vehicles, creates the need for smart home energy management systems that make use of sophisticated data analytics solutions, including (net) load forecasts. As a consequence, the number of published research articles in this field has been growing strongly, and methods are becoming increasingly complex and specialized. To identify the state of the art of forecasting individual households' electricity consumption, this chapter qualitatively reviews high impact studies in this field, thus identifying best performing methods, best practices, and promising pathways for future research.[18]

[18] In this thesis, the terms "consumption forecasting" and "load forecasting" are used interchangeably.

To achieve these goals, this chapter builds on the comprehensive literature review of data analytics in the electricity sector conducted by vom Scheidt et al. (2020). Section 7.2 introduces the dimensions along which the reviewed studies are categorized. In Section 7.3, the methodology used for searching and selecting relevant articles is outlined. Then, catering to the focus on this thesis, the level of analysis is narrowed to the category of "short-term forecasting of individual loads" and a structured in-depth review of the most influential studies in this category is given in Section 7.4. In Section 7.5, the review findings are summarized and best practices for the design of forecasting models in the context of smart home energy management systems are derived.

7.2 Dimensions of Analysis

The review is structured along three dimensions: *area*, *application* and *approach*, which are described in more detail in the following.

7.2.1 Area

The electricity system value chain can be structured into the following components: (i) Generation, (ii) Trading, (iii) Transmission and Distribution, (iv) Consumption, and (v) System. Generation refers to the transformation of other forms of energy to electric energy. Trading refers to the buying and selling of electricity on wholesale or retail markets. Transmission and Distribution denotes the delivery of electricity via grids. Consumption is the demand and end-usage of electricity. Studies that contemplate the system as a whole and simultaneously assess multiple areas are grouped in the System area.

7.2.2 Application

This chapter defines application as the specific task or activity on which an investigation focuses. Based on typical applications from Data Analytics literature, four categories are defined: (i) Forecasting and Prediction (Supervised Data Analytics), (ii) Clustering (Unsupervised Data Analytics), (iii) Monitoring and Controlling (both supervised and unsupervised), and (iv) Other. Forecasting and Prediction are both concerned with the estimation of outcomes for unseen data. In addition, because the terms 'prediction' and 'forecasting' are used as synonyms by many authors, the first category comprises both applications. Clustering, on the other hand, is the aggregation of objects into homogeneous groups. As for Monitoring and Controlling, both terms are related and involve a process of observation and measurement of performance in order to take corrective action, if necessary.

7.2.3 Approach

To compress the exceptionally large amount of single and combined methods existing in Data Analytics research, this review defines eight groups of approaches that represent the third perspective of analysis of each reviewed paper: (i) Time Series, (ii) Regression, (iii) Neural Network, (iv) Support Vector Machine, (v) Tree based Approaches, (vi) Clustering Approaches, (vii) Hybrid Approaches, (viii) Other Approaches, and (ix) literature reviews. This chapter categorizes an approach as Time Series if it falls into one of the following families: autoregressive integrated moving average (ARIMA), generalized autoregressive conditional heteroskedasticity (GARCH), Kalman filtering, Grey system theory, exponential smoothing, or transfer functions. Regression can be defined as an approach used to identify a functional relationship between the explanatory and the dependent variables (Mat Daut et al., 2017). Apart from the support vector regression (SVR) and the regression tree, all types of regressions – including linear, logistic, logic, and quantile regression – belong to this category. Artificial Neural Networks (ANN) are Machine Learning approaches inspired by cells in the human brain. Similar to brain neurons, artificial neurons are connected with each other in multiple layers, forming a network Mat Daut et al. (2017). The network can adopt multiple architectural forms. The Support Vector Machine (SVM) is a Machine Learning approach for classification and regression problems (Mat Daut et al., 2017). When used for regression, it is known as SVR. Tree based approaches function by developing a tree to predict an output from input variables. They can be used for classification and regression. Related approaches are, e.g. random forests, boosting and bagging as well as Extra Trees. Clustering approaches aggregate objects in homogeneous groups, in other words, clusters. Two clustering families exist – hierarchical and partitioning approaches. We categorize an approach as a Hybrid if it combines two or more approaches from the classes defined above. This excludes models which use a second approach only for pre-processing. If an approach cannot be allocated to any category, it is defined as Other Approach.

Figure 7.1 gives an overview of the relationships among these three dimensions, together with examples. A typical study considered in this chapter uses real-world data from an area, introduces a certain application use case and presents one or more approaches. The results give new insights on both the respective area and the performance of the approach.

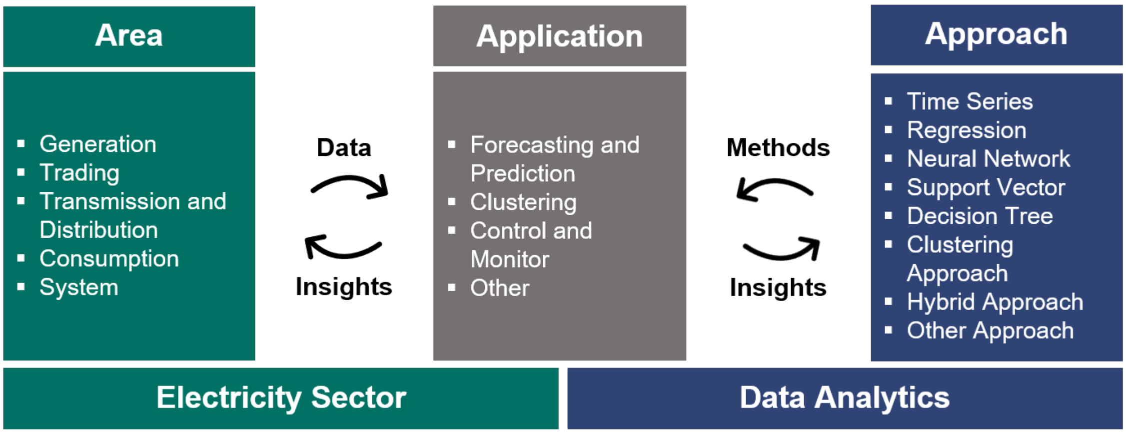


Figure 7.1.: The three dimensions of analysis and their interaction.

7.3 Methodology

In order to identify the main streams of relevant literature, we follow the fundamental three steps suggested by Webster and Watson (2002): (1) identify major contributions, (2) search backwards, and (3) search forwards. The scope of the original review (vom Scheidt et al., 2020) is very broad compared to other review articles. Therefore, we enhance the conventional first manual step of identifying major contributions with a database query search and automatic filtering based on data mining. Our methodology is presented in detail below to ensure transparency and validity. Figure 7.2 gives an overview of the steps described in this section.

7.3.1 Selection of Initial Paper Pool

The starting point for identifying literature for the review is a manual selection of highly relevant papers. Selection is performed with the help of experts in the field, taking into account the number of citations of a paper and the journal rank

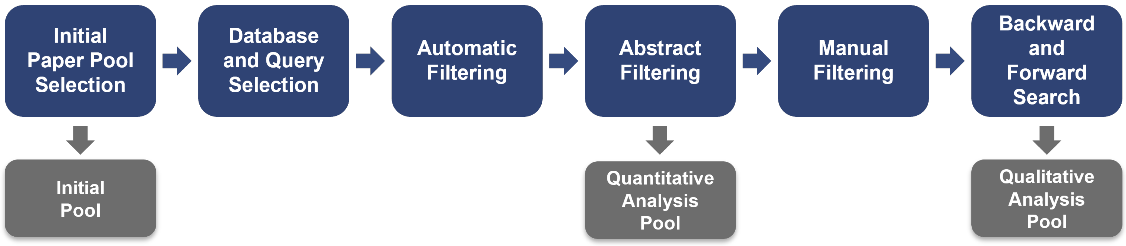


Figure 7.2.: Overview of the methodology used for searching and selecting relevant papers.

in terms of h-index and impact factor. The result of this step is the Initial Pool, consisting of 50 studies (see references Ahmad (2017); Almeshaiei and Soltan (2011); Amjady (2001, 2006, 2007); Azadeh et al. (2008); Biscarri et al. (2017); Mabel and Fernandez (2008); Catalão et al. (2007); Chicco (2012); Chicco et al. (2006); Conejo et al. (2005); Figueiredo et al. (2005); Foley et al. (2012); Gross and Galiana (1987); Haben et al. (2016); Hong et al. (2016); Hong and Fan (2016a); Hong and Hsiao (2002); Hor et al. (2005); Hyndman and Fan (2010); Kalogirou (2001); Kankal et al. (2011); Kavaklioglu (2011); Kaytez et al. (2015); Keles et al. (2016); Khuntia and Panda (2012); Kwac et al. (2014); Lago et al. (2018); Nagi et al. (2010); Nizar et al. (2008); Nogales et al. (2002); Pappachen and Peer Fathima (2017); P. Gross et al. (2006); Reikard (2009); Sfetsos and Coonick (2000); Shayeghi et al. (2007); Sidhu et al. (1995); Singhal and Swarup (2011); Staudt et al. (2018b); Suganthi and Samuel (2012); Szkuta et al. (1999); Tascikaraoglu and Uzunoglu (2014); Taylor and McSharry (2007); Tso and Yau (2007); Viegas et al. (2017); Voyant et al. (2017); Weron (2006, 2014); Zhou et al. (2010)).

7.3.2 Evaluation and Selection of Most Appropriate Database and Query

The second step in capturing high-impact literature for the review is an online database search. To this end, we evaluate different databases and search queries, and select the one best-suited to the purpose. For the database selection, the deciding factor is the number of studies of the initial paper tool it contains. This number must be maximized. We evaluate the established databases Web of Science, Scopus, Science Direct, IEEE Xplore, and Wiley Online Directory. We select Web of Science, because it is the database which contains the highest number of studies, i.e. 44 of the 50 studies listed in the Initial Pool.

Next, a search string is constructed that searches the titles and abstracts of all articles in the respective database. When constructing the search string, three aspects are taken into account: the consistency of the query, the number of papers of the Initial Pool found with it, and the total number of papers retrieved by it. After assessing 10 different queries, a query that best balances the three aspects is selected.

The search string is composed of four parts, which are linked with the logical AND. The first part of keywords refers to the general object of analysis in a paper, such as *electricity*. The second part refers to the area or subtopic, for instance *transmission*. In the third part, the keywords refer to the application of the study, e.g. *load frequency control (LFC)*. Finally, the fourth part consists of approaches that might be used, such as *neural networks*. The keywords within each part are linked with the logical OR.[19]

> (electric* OR energy OR power OR load OR radiation OR "smart meter$" OR lines OR voltage) AND
>
> (customer$ OR consum* OR demand OR generation OR transmission OR distribution OR retail OR "short term" OR "long term" OR loss* OR stability OR system$ OR solar OR price$) AND
>
> (cluster* OR segment* OR forecast* OR predict* OR detect* OR analy* OR simulat* OR applicat* OR implement* OR monitor* OR control* OR characteriz* OR "LFC") AND
>
> (technique$ OR model OR data OR "artificial intelligence" OR "learning machine" OR "machine learning" OR "time series" OR "regression analysis" OR "decision tree" OR "neural network$" OR "ANN" OR "support vector" OR "deep learning" OR "data mining" OR "ARIMA" OR "ARMA" OR "ANFIS")

The search is performed using the selected string on the chosen database in February 2019. In total, 7,708 papers are retrieved.

[19] $ indicates that a keyword can be singular or plural. * is a placeholder for any combination of letters; "consum*" e.g. captures "consumer" and "consumption".

7.3.3 Automatic Filtering

Of the retrieved articles, those most relevant and suited are identified using a text mining algorithm. The algorithm's goal is to determine the most relevant documents in relation to the given search query and it is implemented using the programming language R.

Firstly, the search string is disaggregated into a list of 20,834 queries that contains all possible combinations resulting from the selection of one keyword per category block of the aggregated query. Secondly, a Vector Space Model is constructed, using the disaggregated search strings and the abstracts of the 7,708 documents retrieved in the previous step. The Vector Space Model is an algebraic model that involves two steps: the representation of each document as a vector of the words that occur within it and the transformation of the vectors into a numerical format. When breaking the documents into vectors, preprocessing steps are applied in order to remove stop words, numbers, any extra white spaces and punctuation, and to reduce the remaining words to their word stem. For the second part of the Vector Space Model, a Term Document Matrix is constructed. This is a method of representing document vectors in a matrix format, where rows stand for all the terms present in at least one of the documents, and columns represent the document vectors across all terms. In this case, a cell value in the matrix is filled with the number of times the particular term is present in the particular document. If the term is not present in the document, then the cell value contains the number 0.

We define articles as relevant when they have a high similarity to the search string. Because documents and queries are represented as vectors, the angle θ between the vectors can be used as a similarity measure. The cosine similarity between two documents on the Vector Space is a measure that calculates the cosine of the angle between them, according to 7.1.

$$similarity = \cos(\theta) = \frac{AB}{\|A\|\|B\|} = \frac{\sum_{i=1}^{n} A_i B_i}{\sqrt{\sum_{i=1}^{n} (A_i)^2}\sqrt{\sum_{i=1}^{n} (B_i)^2}} \tag{7.1}$$

This metric is a measure of orientation and not magnitude, since it focuses on the angle between the documents, and not the magnitude of each word count. In this sense, the cosine similarity is advantageous because even if two similar documents are far apart according to the Euclidean distance - due to the difference in size - they will still be oriented close together. However, a document containing only the words from a string vector several times will not be closer to that vector than a document with the same words appearing just once.

After the calculation of the cosine similarity between each paper vector and each search string vector, each document is assigned its highest obtained score, i.e. the highest cosine similarity obtained with any of the string vectors. As a result of this first step of filtering, the top 1,000 papers with the overall highest similarity score are selected.

7.3.4 Abstract Filtering

A second manual step of filtering is performed by reading and evaluating the abstracts of the top 1,000 documents. Firstly, we exclude studies which use only physical or engineering methods. In addition, we rule out studies that cover the application of Data Analytics in an energy sector that does not include electricity. Following this step, 514 papers remain, which form the Quantitative Analysis Pool depicted in Figure 7.2 used to carry out the quantitative analysis of electricity analytics research.[20] The pool is later refined for the qualitative analysis, as described in the paragraphs below.

7.3.5 Manual Filtering

In order to conduct a qualitative analysis of the studies in this area, a more fine-tuned pool of literature is needed. With this objective, the papers are grouped by area and year. Within each group, they are then ordered according to their number of citations. The amount of studies to select from each group is defined according to the proportion that each one represents in relation to the Quantitative Analysis Pool. The grouping thus has two purposes: to control the influence that the year of publication has on the number of citations, and to ensure that the proportion of articles in each area remains the same as before. Based on these criteria, the documents with the highest number of citations are selected from each group. Following this second step of filtering, 147 studies remain.

[20]See vom Scheidt et al. (2020).

7.3.6 Backward and Forward Search

To ensure that the most relevant literature is analyzed, backward and forward searches are conducted. The backward search is the revision of papers cited by the articles that are currently part of the literature list, thus determining prior studies that also should be included. The forward search, on the other hand, is the identification of papers that cite the articles that are included in the literature list, thus determining subsequent studies that should be included. As part of the backward search, all papers that are cited by at least 10 of the articles on the current literature list are included. Following this step, 9 new studies are added to the list. For the forward search, papers that cite the articles on the current literature list, and have an above average number of citations in relation to them, are included. In the course of this step, 16 new studies are added to the list. Finally, the literature list is merged with the Initial Pool, excluding duplicates.

The resulting Qualitative Analysis Pool includes a total of 205 studies. Of these 205, 24 are categorized into the category “Short-term forecasting of individual consumption”. The review of these studies is presented in Section 7.4. For qualitative reviews of studies in the other areas, and quantitative analyses of the paper pool, the interested reader is referred to vom Scheidt et al. (2020).

It should be noted that due to the broad scope of the attempted review, we concentrate on the most important studies and fields of research with the highest impact. Other studies related to *Data Analytics in the electricity sector* exist, but have not been at the center of discussion at the time the review was conducted.

7.4 Qualitative review of short-term forecasting of individual consumption

In an electricity system with multiple distributed technologies such as rooftop solar PV panels, home battery storage, smart meters, and controllable smart home appliances, the need as well as options for forecasting individual consumption increase compared to the status quo. Potential use cases are efficient building operation and optimization Deb et al. (2017) as well as smart storage operation. Compared with system-wide forecasting, the forecasting of individual consumption is a more recent stream of research. We classify 13 studies, plus eleven reviews in this category. All studies forecast the total consumption of households in a given time interval for a short-term horizon. Fan et al. (2014) also forecast daily peak values.

7.4.1 Approach overview

Most high-impact studies that forecast short-term individual consumption use ANN (Kalogirou, 2000, 2001; Neto and Fiorelli, 2008; Zhao and Magoulès, 2012; Quilumba et al., 2015; Cai et al., 2019; Ahmad et al., 2018) or ANN based hybrid approaches (Zhao and Magoulès, 2012; Fan et al., 2014; Ahmad et al., 2014; Li et al., 2015; Dong et al., 2016; Deb et al., 2017; Mat Daut et al., 2017; Muralitharan et al., 2018; Li et al., 2018; Almalaq and Zhang, 2019). In addition, SVR (Jain et al., 2014; Ahmad et al., 2014; Dong et al., 2016; Zhang et al., 2016; Mat Daut et al., 2017; Ahmad et al., 2018), SVR based hybrid approaches (Mat Daut et al., 2017), and Bayesian Networks (Singh and Yassine, 2018) are used.

7.4.2 Data sets

The data for these studies come from office buildings (Neto and Fiorelli, 2008), residential buildings (Jain et al., 2014; Quilumba et al., 2015; Dong et al., 2016; Singh and Yassine, 2018; Almalaq and Zhang, 2019), commercial buildings (Li et al., 2018; Cai et al., 2019), public sector buildings (Li et al., 2015; Zhang et al., 2016; Almalaq and Zhang, 2019; Cai et al., 2019), private BEVs (de Cauwer et al., 2015), and mixed-use buildings (Fan et al., 2014). Most studies use one type of data set to evaluate their method. The length of the time series used varies depending on the study and ranges from ten days (Zhang et al., 2016) to five years (Almalaq and Zhang, 2019). Time granularity of data is usually between 15 minutes and one hour. Several studies utilize very granular consumption data in the range of one to five minutes (Almalaq and Zhang, 2019; Singh and Yassine, 2018; Dong et al., 2016). Notably, Singh and Yassine (2018) use appliance-level data measured at six-second intervals. Available data sets are usually split up into training and test sets and sometimes an additional validation set. Typically, training sets contain 60-80% of the data. The largest training set share is used by Cai et al. (2019) with 90%. In general, accuracy tends to increase with the training set – in (Singh and Yassine, 2018) for example from 82% at 25%, to 86% at 50%, and 90% at 75%. Compared with *system-wide* consumption forecasting, training set shares tend to be larger. This might indicate additional difficulty in forecasting *individual* consumption.

7.4.3 Feature selection

All forecasting studies that focus on buildings use historical consumption data as an input feature. Multivariate models utilize additional external variables as input features. The most common are temperature-related (6), followed by type of day (4), month or season (4), and solar radiation (3). When using external variables, studies should ensure that only information is used that in reality would be available at the time of forecasting. This aspect poses a notable limitation to the study by Cai et al. (2019), which uses actual "future" weather data as an external input, and not the weather forecast. The authors add "white noise" cases for robustness analysis, but this still assumes that weather forecasting errors follow a Gaussian distribution, which impacts practical usability. We recommend choosing one of three other methods to integrate weather data in consumption forecasts, in line with Hong et al. (2016). Forecasters could either (a) use historical weather *forecasts* directly, (b) rearrange the original historical weather data with e.g. bootstrap methods, or (c) create a mathematical weather forecasting model and use its output as input for the consumption forecast.

The BEV forecasting study (de Cauwer et al., 2015) represents a special case, as it does not use historical consumption data as input, but instead relies on kinematic parameters of trips – such as distance, travel time, and temperature – and cars – such as acceleration.

In general, a higher number of features tends to improve forecasting accuracy, but also the risk of over-fitting. Some studies pay special attention to feature selection. Neto and Fiorelli (2008) employ Recursive Feature Elimination for feature selection. Li et al. (2015) utilize principal component analysis. Cai et al. (2019) and Fan et al. (2014) select external features based on the Pearson Correlation Coefficient and the Coefficient of Determination of feature values and consumption values, respectively. Another promising approach is to utilize variables from similar surrounding buildings via cross correlation, or mutual entropy methods (Yildiz et al., 2017).

7.4.4 Benchmark approaches

All building forecasting studies benchmark their proposed approach against others. Benchmarks can range from naive baseline persistence models to more advanced physical, statistical and Machine Learning approaches. Notably, some studies compare a wider selection of approaches from different categories (Fan et al., 2014; Dong et al., 2016; Almalaq and Zhang, 2019).

7.4.5 Evaluation metrics

The 13 reviewed studies of individual consumption forecasting do not show a common, default error measure. Instead, a variety of measures can be observed, including Mean Absolute Percentage Error (MAPE) (6), Root Mean Squared Error (RMSE) (5), Coefficient of Variation (5), Mean Absolute Error (MAE) (4), and a long tail of twelve other measures. One key reason for this variety is that certain conventional error metrics like MAPE become impossible to calculate when values are zero and very high when values are close to zero – which are likely to occur for individual consumption. The resulting diversity in measures limits the comparability of studies. Therefore, reporting multiple error metrics is advisable. Forecasters should also be aware that MAPE, RMSE, and MAE are point-wise measures, which double-penalize models, which forecast the shape of the consumption curve well, but get the timing wrong. For applications which have a certain tolerance for mistiming, it can therefore be more appropriate to conduct a restricted permutation of the original forecast and select the one that minimizes the error (Yildiz et al., 2017). Last, probabilistic forecasts demand new evaluation metrics. The *pinnball loss function* has seen widespread use and provides easy implementation and communication (Hong et al., 2016).

7.4.6 Complexity and running speed

Only few studies explicitly state the complexity and computational efficiency of their models. In the reported cases, most models can be trained and run in a matter of minutes on standard personal computers. Nevertheless, the time needed for building and training models can vary substantially. For training, times might vary between two seconds and five minutes depending on the approach Fan et al.

(2014). Similarly, comprehensive feature selection takes additional time – Fan et al. (2018) report between nine seconds and 50 minutes. On the upside, reducing the number of features can decrease training time of the model. In ensemble models, the weighting step takes additional time.

As the computational and modelling effort can be highly significant in real-world use cases, authors are encouraged to report them. Furthermore, authors who wish to demonstrate the usability of their approaches for real-time applications are encouraged to report training times.

7.4.7 Notable approaches

Firstly, it has been shown that ANN models can perform better when trained separately for working days and non-working days, i.e. weekends and holidays. The ANN models in Neto and Fiorelli (2008) achieve average errors of 10.8 (working days) and 10.5 (non-working days) compared with 21.0 for a combined model.

Secondly, hybrid approaches tend to outperform their individual component approaches both for total energy consumption and peak power forecasting (Fan et al., 2014; Almalaq and Zhang, 2019). On the downside, hybrid approaches demand higher computational and modelling effort. This should be weighted against the gains in accuracy, especially when those gains are minor, as reported by Zhang et al. (2016).

Thirdly, current Deep Learning Approaches such as Deep Belief Networks can outperform many advanced approaches such as ANN, ELM, and SVR (Li et al., 2018; Amasyali and El-Gohary, 2018).

7.4.8 Summary

In decentralized electricity systems, forecasting short-term consumption at a distributed level gains importance. This new challenge can be tackled with tailored solutions, as the various approaches reviewed in this section show. The selected forecasting time horizon can influence the suitability of approaches (Muralitharan et al., 2018). The state-of-the-art in short-term forecasting of individual consumption includes careful feature selection, hybrid approaches and deep learning approaches, all of which come at higher modelling and computation costs than conventional approaches, which must be weighted against accuracy improvements for each use case.

In comparison with *system-wide* consumption forecasting, no studies use ARIMA based models, training sets tend to be larger, and more attention is awarded to feature selection. When used as benchmarks, ARIMA based models are outperformed by others. This suggests that ARIMA based models might be less suitable for capturing the higher volatility in *individual* consumption profiles. The larger training sets and more sophisticated feature selection methods indicate higher requirements of *individual* consumption forecasting.

In addition, no default error measures exist. We propose using the mean absolute scaled error (MASE), as it does not rely on division by the actual consumption value – and thus is very suitable for individual consumption values, which can be close to zero at times –, enables comparability across data sets and scales, penalizes positive and negative errors equally, and can be easily interpreted. In cases, where large errors in forecasting lead to over-proportionally large losses it is adequate to also report non-linear loss metrics like the root of the average squared error. For applications, where the shape of the consumption curve is more important than the timing, we propose conducting a restricted permutation of the original forecast, and selecting the error minimizing forecast.

Most studies use one type of data set to evaluate their method, which limits the generalizability of their findings. We therefore encourage authors to a) assess various approaches, b) apply their model to a reference data set, which has been used by other studies in the past, c) report accuracy, computational setup and running time as well as model building effort, and d) calculate and present multiple common error measures for evaluation. This way, future studies can provide valuable new insights for the forecasting community and foster convergence of research in this field.

The field of peak consumption forecasting is relatively small and offers future potential, for example with respect to demand response, as electricity tariffs with peak demand and peak capacity charges gain attention (Burger et al., 2019). For this and further use cases, probabilistic forecasting can be expected to play a large role as individual consumption exhibits higher volatility and uncertainty than system-wide consumption.

7.5 Conclusion

The presented review reveals multiple key takeaways for the development of a state of the art forecasting model. First, for high performance, Machine Learning models, and probabilistic approaches appear favourable compared to conventional statistical methods and non-probabilistic models. Second, features should be selected carefully and tailored to the problem context. Third, for research rigour, various approaches should be developed and compared on the same data set, public reference data sets should be used, and common error measures should be used. These key findings motivate the design of a novel forecasting model that is presented in Chapter 8.

CHAPTER 8

LOAD FORECASTING FOR INTEGRATED HOME ENERGY SYSTEMS

Roof-top solar PV plants, residential electric heating, and other distributed energy technologies, together with time-varying tariffs, create demand for smart home energy management systems. These systems rely on accurate forecasts of electricity generation and consumption in order to calculate optimized operation schedules for all technologies. In recent years, first probabilistic load forecasting models for households have been developed, with growing model complexity and performance. In comparison to point forecasts, probabilistic models provide more information about future uncertainties (Wang et al., 2019), and thus can be more useful for smart home energy management systems. However, past probabilistic forecasting research has largely ignored the influence of new technologies on forecasts. To address this important gap, this chapter presents a dedicated net load forecasting model for households with solar PV plants, electric heating, or both.

Informed by the review conducted in Chapter 7, a probabilistic forecasting model based on an Artificial Neural Network with Gated Recurrent Units (GRUs) is developed. The model specifically uses data from weather forecasts as external features, in contrast to the commonly used actual weather data. Further following best practices of assuring comparability and replicability, the model is applied to an openly available data set, and compared to three benchmark models. The results show that a quantile Long Short-term Memory (LSTM) model from literature performs best for households without the aforementioned technologies, but the proposed quantile GRU model performs best for households with solar PV plants, electric heating, or both. In general, forecasting losses are lowest for households with solar PV, and highest for households with electric heating. These findings lead to the conclusion that the increasing adoption of distributed energy technologies is likely to affect the quality of existing forecasting tools.

This chapter comprises the published article: F. vom Scheidt, X. Dong, A. Bartos, P. Staudt, C. Weinhardt, *Probabilistic Forecasting of Household Loads: Effects of Distributed Energy Technologies on Forecast Quality*, Proceedings of the Twelfth ACM International Conference on Future Energy Systems, 2021.

8.1 Introduction

In electricity systems with increasing numbers of distributed energy technologies (DETs), appropriate short-term forecasting of load at a granular level gains importance (Wang et al., 2019; vom Scheidt et al., 2020). Probabilistic load forecasting models for households provide more information about future uncertainties than point forecasts (Wang et al., 2019), but have been focused on 'conventional' residential load, and have largely neglected the influence of distributed energy technologies. Therefore, this chapter makes the following contributions: First, it provides a new semi-synthetic residential data set, which contains the net load profiles of 40 households, differentiated by heating type (electric space heating, no electric space heating), and rooftop solar PV installation (solar, no solar). This unique data set is used to analyze how well probabilistic forecasting models perform over various types of households with DETs. Second, it presents a probabilistic forecasting model based on Gated Recurrent Units that includes data from weather forecasts and calendar variables as external features. This model is compared to three benchmark models, one of them a recently proposed model based on Long Short-term Memory networks (Wang et al., 2019). The chapter thus sheds light on the so-far neglected role of DETs in residential probabilistic load forecasting, proposes a new forecasting model that is compared to state-of-the-art benchmark models, and provides a new benchmark data set for future research in this area.[21]

[21]Code and data are available at `https://github.com/FVS-energy/prob_forecasting`.

8.2 Related work

Unlike point forecasting, which provides a single predicted value at each time step, probabilistic forecasting makes it possible to express the uncertainty in a prediction, which is a crucial component for optimal decision making (Gneiting and Katzfuss, 2014). For electrical load, probabilistic forecasting generates a distribution of the future load, thus capturing characteristics of a load profile's volatility. As suggested by Hong and Fan (2016b), probabilistic load forecasts can be conducted in terms of quantile forecasting, interval forecasting and density forecasting. In recent years, there has been growing interest in probabilistic load forecasting on city level or system level. A structured overview of probabilistic load forecasting studies is provided in Table 8.1. The overview shows that studies have investigated a wide range of new methods, including kernel methods (Arora and Taylor, 2016), neural networks (Elvers et al., 2019; Wang et al., 2019; Van der Meer et al., 2018b; Vossen et al., 2018; Gan et al., 2017), Gaussian process (Shepero et al., 2018; Van der Meer et al., 2018a,b), additive quantile regression (Taieb et al., 2016), and ensemble models (Munkhammar et al., 2021; Afrasiabi et al., 2020). However, most studies have applied these methods to regular households' loads. Regarding household load influenced by DETs, Van der Meer et al. (2018b) address probabilistic forecasting of net loads of houses with rooftop solar PV. They propose a dynamic Gaussian Process that produces sharper prediction intervals at significant lower computational effort than the provided benchmarks. However, there is a trade-off with the ability to capture sharp peaks. The authors also find that indirectly forecasting net demand (i.e. through forecasting both demand and self-generation) leads to wider prediction intervals with higher coverage probability. In a following work, Van der Meer et al. (2018a) find that net load forecasts have improved sharpness and reliability of prediction intervals, when several households are aggregated. This hints at the specific challenges of individual load forecasting. However, neither of the two studies compares households with different technology set-ups. Besides probabilistic household load forecasting, studies have developed specialized probabilistic forecasts for flexibilities of electric vehicles (Huber et al., 2020), or rooftop solar PV generation (Afrasiabi et al., 2020), but without integrating these into residential load forecasts.

In summary, past research has focused on the development of models for household

Table 8.1.: Overview of probabilistic individual load forecasting literature

Study	**Main method(s)**	**Input features**	**Data**	**Evaluation metric**	**Load scenarios**
This study	*GRU, LSTM*	*net load, calendar, weather*	*1 year at 1 h resolution*	*Average pinball loss*	*Household (HH), HH with solar, HH with heating, HH with solar + heating*
Munkhammar et al. 2021	Markov-chain mixture distribution model	load	3 years at 30 min resolution	Reliability MAE, PINAW, normalized CRPS	HH
Afrasiabi et al. 2020	Ensemble of CNNs, GRU, MDN	load, weather	1 year at 30 min resolution	RMSE, MAPE, CRPS, CE	HH
Zhang et al. 2020b	Ensemble of GRU, GBRT, RF, LightGBM	load, calendar	1.5 years at 30 min resolution	CRPS	HH
Elvers et al. 2019	CNN	load, calendar, weather	2 years at 15-60 min resolution	Pinball loss	HH
Wang et al. 2019	LSTM	load, calendar	1.5 years at 30 min resolution	Average pinball loss	HH
Shepero et al. 2018	Gaussian process, log-normal process	load, calendar	3 years at 30 min resolution	MAE, RMSE, PINAW, PICP	HH
Van der Meer et al. 2018a	Static + dynamic Gaussian Process	net load	3 years at 30 min resolution	MAE, MAPE, NRMSE, PICP, PINAW, NCRPS	HH with solar
Van der Meer et al. 2018b	Dynamic Gaussian Process, Quantile regression	net load	3 years at 30 min resolution	PICP, PINAW, NCRPS	HH with solar
Vossen et al. 2018	MDN, Softmax Regression Networks	load, calendar	three different data sets	CRPS	HH
Gan et al. 2017	LSTM	load	500 d at 30 min resolution	Average quantile score	HH
Taieb et al. 2016	Boosting additive quantile estimation	load	1.5 years at 30 min resolution	CRPS	HH
Arora and Taylor 2016	Conditional kernel density estimation	load	8 mo at 30 min resolution	CRPS, unconditional coverage	HH

CE: Cross-entropy, CNN: Convolutional neural network, GBRT: Gradient boosting regression tree, RF: random forest, LGBM: Light gradient boosting machine, CPRS: Continuous Ranked Probability Score, MAE: Mean average error, MAPE: Mean average percentage error, MDN: Mixed density networks, NRMSE: Normalized root mean squared error, PICP: Prediction interval coverage probability, PINAW: Prediction interval normalized average width, NCRPS: Normalized continuous ranked probability score, RMSE: Root mean squared error

load, or specific single technologies. An important gap prevails regarding probabilistic load forecasting for consumers with different types of DETs that are about to "disrupt the traditional load profiles" (Wang et al., 2019).

8.3 Methodology

This section introduces the structure of the proposed forecasting model. Additionally, it describes benchmark methods, the selected loss metric, hyperparameter tuning, and cross-validation.

8.3.1 Long Short-Term Memory Networks and Gated Recurrent Units

Unlike traditional neural networks, which learn the relationships of inputs and outputs based on provided training data for every instance, recurrent neural networks (RNNs) are able to learn dependencies within sequential input data such as time series. However, conventional RNNs can practically only learn short-term dependencies due to the problem of vanishing gradients. As a remedy, LSTM networks have been developed, which are able to learn long-term dependencies (Hochreiter and Schmidhuber, 1997; Gers et al., 1999). There are three gates in an LSTM unit, which control the flow of information in the network. However, LSTMs can suffer from slow training since parameters for three gates have to be estimated.

Compared to LSTMs, GRUs have one less parameter that needs to be estimated. In other contexts, GRUs have shown similar performance as LSTMs, with shorter computational times (Chung et al., 2014; Ke et al., 2019). Therefore, in this chapter, we present a probabilistic forecasting model based on quantile forecasts with GRUs.

The inner structure of a GRU unit is illustrated in Figure 8.1. The two gates of a GRU are called update gate z_t and reset gate r_t. The update gate z_t controls how much information from the previous state should be passed in the future. It is determined by the hidden state of the last time step h_{t-1} and the current input h_t, as shown in Equation 8.1. Similarly, the reset gate r_t controls, which information from past steps should be forgotten, as shown in Equation 8.2. A candidate hidden state $\tilde{h_t}$ stores relevant previous information using a reset gate (Equation 8.3). Last, the current hidden state h_t is determined, denoting what information should be passed from the candidate hidden state. h_t is calculated as shown in Equation 8.4.

$$z_t = \sigma(W_z \cdot [h_{t-1}, X_t]) \tag{8.1}$$

$$r_t = \sigma(W_r \cdot [h_{t-1}, X_t]) \tag{8.2}$$

$$\tilde{h_t} = tanh(W \cdot [r_t \cdot h_{t-1}, X_t]) \tag{8.3}$$

$$h_t = (1 - z_t) \cdot h_{t-1} + z_t \cdot \tilde{h_t} \tag{8.4}$$

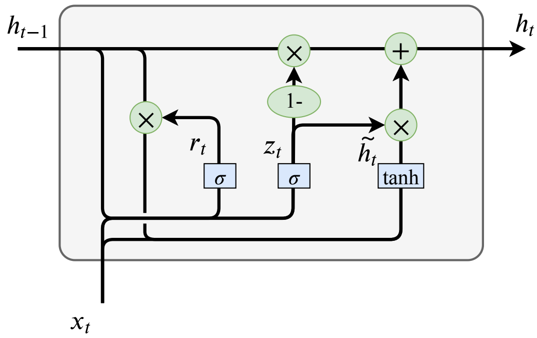


Figure 8.1.: Inner structure of a GRU unit

8.3.2 Network structure

The quantile GRU model (QGRU) includes four steps. A visual representation is displayed in Figure 8.2.

The first step takes historical load data as input. t refers to the predicted time step. n_i is the number of input steps, i.e. the length of the input time series. n_o denotes the number of output steps, defining the prediction horizon. The previous load profile goes through two GRU layers and one dense layer. This layer passes on the last hidden state h_t. In the second step, the calendar data, i.e. the features weekday and time of day, are one-hot encoded. In the third step, weather data are introduced. Each variable, i.e. temperature, wind speed, and relative humidity, is normalized. The fourth step concatenates the output of the three previous steps. Then, the resulting input vector is passed through two fully-connected dense layers, which finally generate five quantile forecasts.

8.3.3 Pinball loss for quantile forecasting

Pinball loss is an established evaluation metric for probabilistic forecasts in the energy sector. It is used as the single deciding error measure in the Global Energy Forecasting Competition (Hong et al., 2016), as well as in studies on probabilistic household load forecasting (Wang et al., 2019; Elvers et al., 2019). Pinball loss evaluates the forecasts of each quantile individually, as formulated by Equation 8.5. The core idea of the pinball loss is the asymmetric penalization of forecast errors, depend-

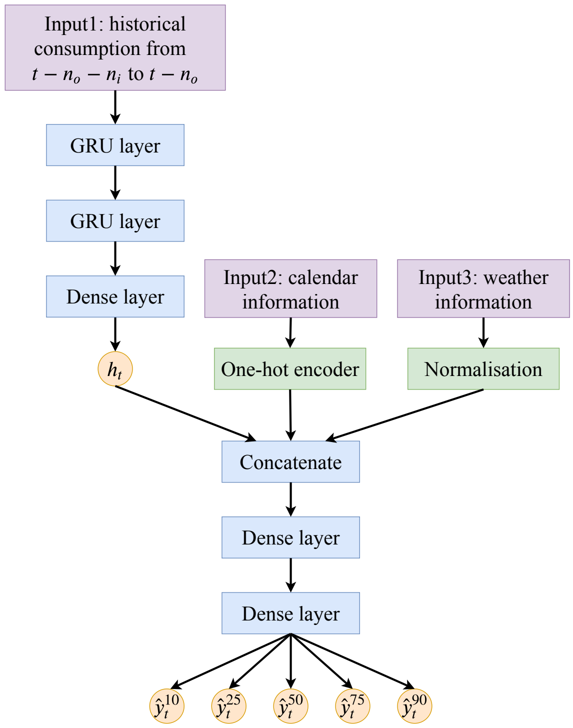


Figure 8.2.: Network structure of the QGRU forecasting model

ing on the quantile. This is represented in Figure 8.3. If a forecasted quantile value is smaller than the actual observation, it is penalized stronger for higher quantiles, as the quantile loss is the product of the quantile and the absolute error. The proposed QGRU model (and all benchmark models) predict five values at each time step for $q \in [10\%, 25\%, 50\%, 75\%, 90\%]$. The aim of the training process is to minimize the average pinball loss of all five quantiles, as formulated by Equation 8.6.

$$L_{q,t}(y_t, \hat{y}_t^q) = \begin{cases} (1-q)(\hat{y}_t^q - y_t), & \hat{y}_t^q \geq y_t \\ q(y_t - \hat{y}_t^q), & \hat{y}_t^q < y_t \end{cases} \tag{8.5}$$

y_t: real observation at time step t
$\hat{y}_t^q$: the qth quantile forecast at time step t

$$minL = \sum_q \sum_{t=1}^{T} L_{q,t}, q \in [10\%, 25\%, 50\%, 75\%, 90\%] \tag{8.6}$$

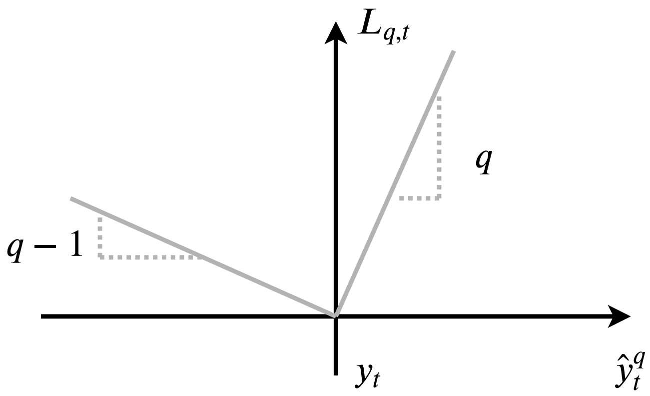


Figure 8.3.: Pinball loss. Own depiction, based on Wang et al. (2019)

8.3.4 Benchmarks

To adequately evaluate the performance of the proposed model, we compare it to three other quantile load forecasting models. The first benchmark is a quantile LSTM (QLSTM) model. It employs LSTM layers instead of GRU layers and thus has the same network architecture as the QGRU model and the same modelling effort. The second benchmark is a quantile regression neural network (QREGNN) model with four dense layers. Both QLSTM and QREGNN take the same input features as the QGRU. We use these two benchmarks to evaluate the QGRU's performance against other models using the same input data. The third benchmark is a quantile LSTM model that does not use weather input features (QLSTM_noWeather). It corresponds to the model proposed by Wang et al. (2019). We use it to measure how the weather features affect the forecast loss and to provide an established benchmark. For all three benchmark models, hyperparameter tuning and cross-validation are performed, to allow for an adequate comparison.

8.3.5 Hyperparameter tuning

Since there are individual models for each household, hyperparameter tuning is done for each model individually. For QGRU, QLSTM, and QLSTM_noWeather, we tune the learning rate, the number of units in the recurrent layers and the number of units in the dense layers. For the QREGNN, we tune the learning rate and the number of units in the dense layers. The tested values are shown in Table 8.2.

Table 8.2.: Values of Hyperparameters

Hyperparameter	**Values**
Learning rate	0.001, 0.01, 0.1
Number of units in recurrent layers	4, 8, 12
Number of units in dense layers	10, 30, 50

8.3.6 Cross-validation

Due to the time series character and the limited time range of the data (one year), a two-fold rolling window approach is conducted to cross-validate the models. First, we train, validate and test our models only on the first 80% of data, i.e. with a train-validation-test split of 40-20-20. Second, we expand the training window, resulting in a 60-20-20 split. For the final evaluation, we average the test losses from step one and two. Rolling window cross-validation is a common approach in energy forecasting (Huber, 2020; Van der Meer et al., 2018b). It improves the generalisation of our findings, amongst others because it better captures seasonality effects.

8.4 Data

This section introduces the data pre-processing steps and the final input data set for the load forecasting task.

8.4.1 Load data

The residential electricity load data was collected by Commonwealth Edison (ComEd), a large electric utility in the US (Exelon, 2018). The data set contains anonymous smart meter data of residential customers in and around the city of Chicago for the year of 2016. Each smart meter provides half-hourly load data, which leads to 16,128 observations for every household. For each customer ID, the delivery service class is stated, which describes the housing type (single family homes and multi family homes), as well as the heating type (electric space heating and no electric space heating). For more information and other applications of the original data set, we refer to Burger et al. (2020) and vom Scheidt et al. (2019). For our purpose, we focus on households in single family homes. From those, we randomly draw ten customers with electric space heating and ten without electric space heating.

8.4.2 Solar data

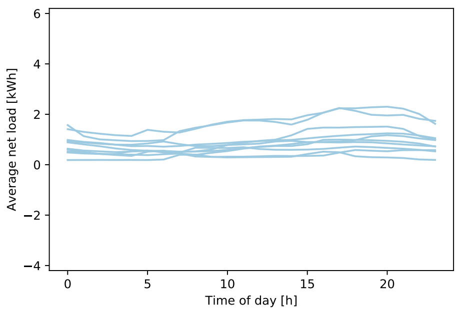
For solar PV data, we use the Python tool pvlib Holmgren et al. (2018). Following the approach from Burger (2019) and Brown and O'Sullivan (2020), we simulate power generation from rooftop solar PV systems based on given weather and irradiation data from 2016. We simulate PV systems with three different azimuths of 135 (south-east), 180 (south), and 225 (south-west) degrees. Each solar PV system is sized to a capacity of 6.9 kW, following Feldman et al. (2021). We randomly assign an azimuth to each household. The assigned solar generation curve is subtracted from the load curve, resulting in the net load. As the forecasts are meant to serve as an input for smart home energy management systems, the forecasts are targeted at the original net consumption of households *prior* to any potential demand response.

Finally, the data set comprises the net load data for 40 households, i.e. for ten households without electric space heating or solar PV (Figure 8.4a in the appendix), for ten households with electric space heating, but no solar (Figure 8.4b), for ten households without electric space heating, but solar (Figure 8.4c), and for ten households with both electric space heating and solar (Figure 8.4d).

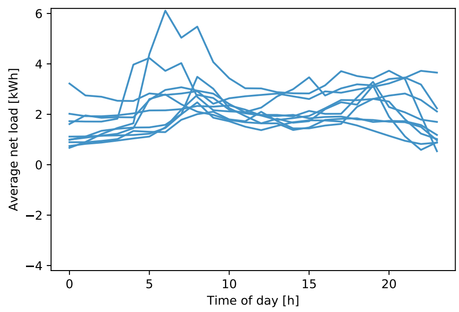
8.4.3 Weather data

When using external input features for forecasting, it should be ensured that only data are used that in reality would be available at the time of forecasting (vom Scheidt et al., 2020). It has been shown that the errors inherent in weather forecasts increase load forecast errors on system level (Alireza Khotanzad et al., 1997). Therefore, we acquire historical weather forecast data for 2016.

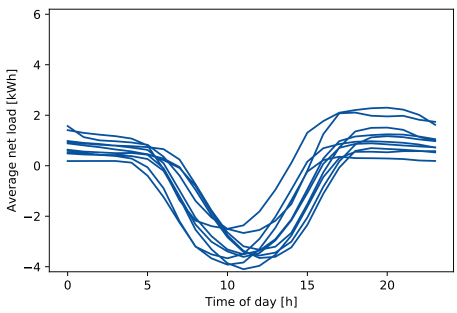
The US "National Oceanic and Atmospheric Institute" provides historical weather forecasts with a sufficiently long history via the Climate Forecast System Version 2 (Saha et al., 2014). In this data base, forecasts for more than 50 variables are stored in six hour intervals. We select air temperature, specific humidity and wind speed, since they are the most frequently used weather variables for load forecasting (Feinberg and Genethliou, 2005) and have a large influence on thermal comfort (Hippert et al., 2001), which presumably plays a crucial role for the load forecasts of households with electric heating. The data sets are provided via a HTTPS file server (National Oceanic and Atmospheric Institute, 2019). From this server, the data can



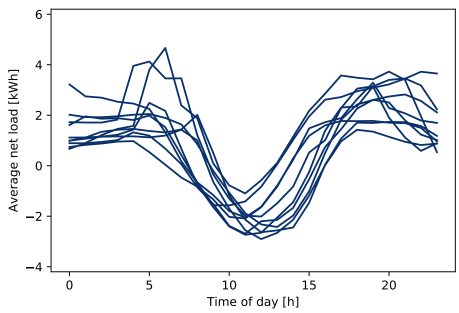
(a) HH with no technology



(b) HH with electric heating



(c) HH with solar



(d) HH with electric heating and solar

Figure 8.4.: Average daily net load curves of the ten households in each group

be downloaded in the Grib2 format and transformed for use in the forecasting task with the Python Package cfgrib. The grid node with the closest spatial proximity to the smart meter area is selected (42.05°, -87.2°). Last, we interpolate the data to hourly values using a cubic regression spline as proposed by Hyndman and Fan (2010).

8.4.4 Calendar data

Electricity consumption patterns on public holidays are usually different from normal days (He, 2017). Past studies have either simply considered all public holidays as weekends (Lusis et al., 2017) or used more sophisticated rules to label public holidays and surrounding days (Hong et al., 2013). We follow the latter approach and re-label special days according to the rules outlined in Table 8.3.

Table 8.3.: Modification of Special Days

Original weekday	Date	Special day	New label
Friday	2016-01-01	New Years Day	Saturday
Saturday	2016-01-02	after New Years Day	Saturday
Sunday	2016-05-29	before Memorial Day	Saturday
Monday	2016-05-30	Memorial Day	Sunday
Tuesday	2016-05-31	after Memorial Day	Monday
Monday	2016-07-04	Independence Day	Sunday
Monday	2016-09-05	Labor Day	Sunday
Tuesday	2016-09-06	after Labor Day	Monday
Thursday	2016-11-24	Thanksgiving	Saturday
Friday	2016-11-25	after Thanksgiving	Saturday
Monday	2016-12-24	Christmas Day	Sunday
Tuesday	2016-12-25	after Christmas Day	Monday

8.4.5 Final input data set

Since other data are given at hourly intervals, the smart meter data sets are aggregated from a half-hourly to an hourly resolution, resulting in 24 observations per day. The final data set for the case study contains three categorical variables (Customer ID, DET set-up, Date), and six input variables for the forecast (Hourly net load, Weekday, Time of day, Hourly temperature forecast, Hourly wind speed forecast, Hourly relative humidity forecast).

8.5 Case study

For the case study, the net load of the next hour is forecasted.[22] For each of the 40 households, an individual model is trained. The last 336 hours (i.e. two weeks) of net load are used as lagged input features. The proposed models are implemented in Python, using Keras. The models are run on a GPU on Google Colaboratory (Google, 2021).[23]

To provide detailed insights into the performance of the models, Figure 8.5 shows

[22]Depending on the use case, this case study could be extended to further output horizons, such as one-day ahead. Testing and comparing multiple output horizons is outside of the scope of this chapter.

[23]Since the allocation of computing resources in Google Colaboratory is not fully transparent, reporting and comparing run times of the models is futile.

a scatter plot of each household's average pinball loss under QGRU, compared to the benchmark models. The line y=x represents the performance of the QGRU. All points under this line indicate a case in which the QGRU outperforms the respective benchmark model. 67.5% of points are under the line, demonstrating the overall superior performance of the proposed QGRU model. More specifically, the QGRU model outperforms the QLSTM in 60.0%, the QREGNN in 72.5%, and the QLSTM_noWeather in 70.0% of cases.

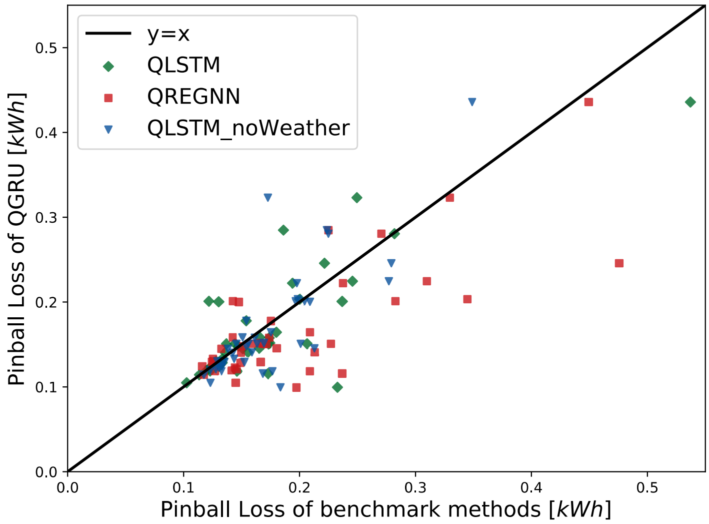


Figure 8.5.: Comparison of pinball loss between QGRU and benchmark models for all customers

In Table 8.4, the performance of the proposed QGRU and the three benchmarks methods, is presented, averaged across customers. The proposed QGRU achieves the lowest pinball losses, overall. It achieves the lowest loss for three of the four customer groups, namely households with electric heating, households with solar PV, and households with both technologies. Only in the case of households without any technology, the benchmark QLSTM model without additional weather input data (as proposed by Wang et al. (2019)) outperforms the QGRU on average. Our results thus confirm the good performance of this model on standard households, but also show that it is outperformed by the QGRU model for households with energy technologies that have atypical electricity net load profiles. This underlines the importance of tailoring forecasting models to the specific case.

Table 8.4.: Average Pinball loss [kWh] of tested methods for different customer types

	QGRU	QLSTM	QREGNN	QLSTM_noWeather	Average
HH	0.1989	0.2019	0.2373	0.1902	0.2070
HH with heating	0.2060	0.2116	0.2602	0.2061	0.2211
HH with solar	0.1366	0.1386	0.1367	0.1387	0.1376
HH with heating & solar	0.1347	0.1394	0.1564	0.1509	0.1453

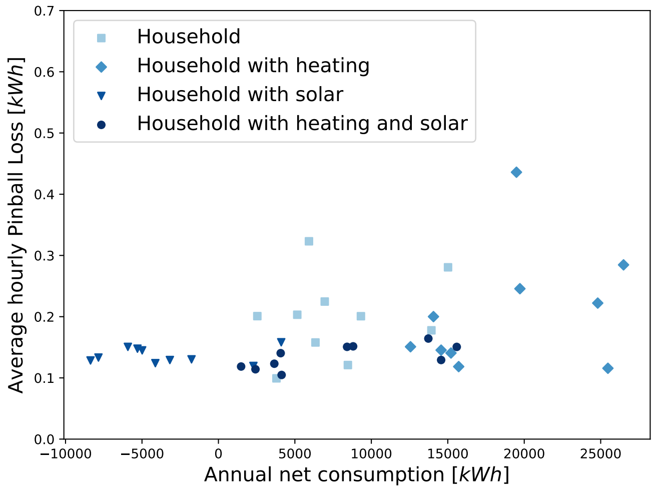


Figure 8.6.: Net load and QGRU pinball loss

All models show the highest average loss for households with electric heating. Figure 8.6 shows the average pinball loss of the QGRU model versus the annual net consumption for each household. The respective figures for the benchmark models can be found in Appendix D. Households with electric heating tend to have higher loads and higher losses. Although differences among models exist, all models show a very high pinball loss for at least one customer from the set of households with electric heating. This finding might indicate that for the tested models, a training set of less than one year, which only includes one heating period is inadequate for learning the households' heating behavior, which is important to consider in the development of future models.

All models achieve the lowest pinball loss on the net load profiles of households with solar generation. Notably, this finding seems to hold independent of these households' total annual net loads, as Figure 8.6 shows. This is surprising and

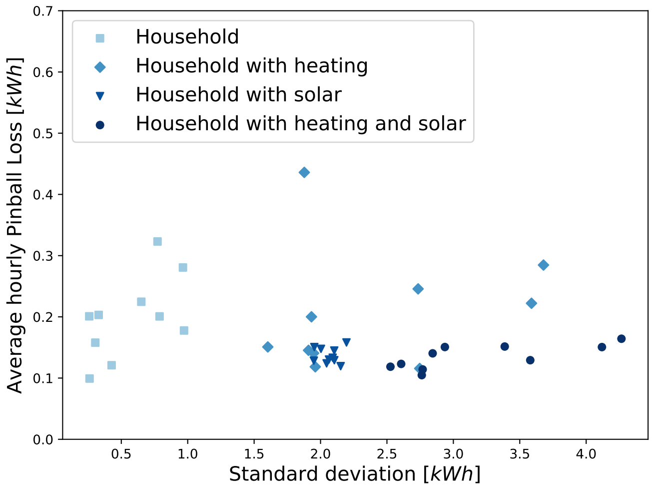


Figure 8.7.: Standard deviation and QGRU pinball loss

indicates that the forecasting models are able to adequately capture the periodicity of net loads that include solar generation. This notion is supported by the comparison of households with no technology and of households with both solar PV and electric heating. These groups have similar mean net consumption, but pinball losses are lower for the latter.

Last, we observe the effect of net load curves' standard deviation on forecast performance in Figure 8.7. Again, the respective figures for the benchmark models can be found in Appendix D. We find that standard deviation is smallest for standard households without DETs and largest for households with both electric heating and solar, reflecting their more variable load curve (see also Figure 8.4d). Notably, the standard deviation does not seem to impact the pinball loss visibly.

Since no literature on probabilistic forecasts of net loads with DET influence exists, we cannot yet benchmark our results against literature. However, we compare our results for households without DETs to Wang et al. (2019), who use a pinball loss guided LSTM without weather data. We find that the QLSTM_noWeather model in our case study achieves an average pinball loss about twice as high as in the case study in (Wang et al., 2019): 0.2019, compared to 0.0963. We assume this difference is due to the higher number of data points per customer in the data set used in Wang et al. (2019): 26,000 data points per customer, compared to 8,783 in our data set.

This indicates the positive effect of more training data on forecasting performance.

Future work could enhance our approach by including other distributed energy technologies, such as electric vehicles and residential batteries. Besides, it can utilize the forecasts by integrating them into the operation of home energy management systems. For this, the code and data published with this study can be used.

8.6 Conclusion

In this chapter, we argue that increasing adoption of distributed energy technologies affects the quality of existing forecasting tools for individual households' net loads. We present a pinball loss guided GRU model that produces quantile forecasts of net loads. We develop a new, semi-synthetic residential net load data set that includes standard customers without distributed energy technologies as well as customers with electric heating, rooftop solar PV, and both technologies. We apply the proposed model and three benchmark models to this data set. We find that the proposed quantile GRU model outperforms the benchmark models for customers with distributed energy technologies, independent of technology. However, the quantile GRU model is outperformed for the group of standard households by a quantile LSTM model that ignores weather data. All models perform best for households with own solar generation, and worst for households with electric heating. We thus provide first fundamental insights for probabilistic forecasting of household load under the influence of distributed energy technologies.

This chapter concludes Part II of this thesis. In this Part, I investigate and evaluate naive and advanced decision support methods for the selection of time-varying electricity tariffs as well as bundles of tariffs and technologies. For the subsequent optimal operation of technologies in response to the tariff, I analyze the state of the art of load forecasting and develop a novel probabilistic forecasting model for residential net loads. Together, these forecasts and decision support methods can facilitate the proliferation of time-varying electricity tariffs and more climate-friendly technologies amongst residential consumers.

The following Part III broadens the scope from electricity tariff engineering for residential customers and the integration of small-scale technologies to tariff effects on the system level and the integration of large-scale technologies, such as electrolyzers.

Part III.

System level

Electricity tariffs do not only have an impact on residential consumers, but also on large consumers in the system. For both the temporal granularity of the electricity tariffs is relevant, as it can incentivize system-beneficial consumption of electricity. Specifically for new, large consumers, the spatial granularity of tariffs is important, too, because it can influence, where in the system the large consumers are being placed. A large key technology that needs to be integrated in electricity systems in the near future, is hydrogen. Hydrogen, produced in electrolyzers with GHG free electricity, is a critical energy carrier for emission reduction in the industry and transportation sectors. Numerous governments are developing support schemes for the scale-up of infrastructure for the production, conversion, transportation, and storage of hydrogen. Since hydrogen electrolysis uses large amounts of electricity, electricity tariffs will have a considerable effect on the setup of this infrastructure and the resulting costs for society. Therefore, it is timely and important to analyze the effects of current tariffs on hydrogen infrastructure and its feedback effects on the electricity grid, as well as to engineer new, more efficient tariffs to foster the integration of hydrogen into the energy system of the future.

CHAPTER 9

EFFECTS OF SPATIALLY DIFFERENTIATED TARIFFS ON HYDROGEN INTEGRATION

In this chapter, the interplay of tariffs on the electricity system level and hydrogen supply chains is analyzed. For this, a novel electrolytic hydrogen supply chain model is developed. This model is then linked to an electricity system dispatch model. For a detailed analysis and case study, two new comprehensive data sets for the German electricity system and the hydrogen demand in 2030 are constructed. Together, this allows the evaluation of the effects of tariffs with spatial and temporal price signals on hydrogen infrastructure, and its feedback effects on the electric system.

This chapter comprises the following published articles and data sets:

- F. vom Scheidt, J. Qu, P. Staudt, D. S. Mallapragada, and C. Weinhardt, *Integrating Hydrogen in Single-Price Electricity Systems: The Effects of Spatial Economic Signals*, Energy Policy, 2022.
- F. vom Scheidt, J. Qu, P. Staudt, D. S. Mallapragada, and C. Weinhardt, *The effects of electricity tariffs on cost-minimal hydrogen supply chains and their impact on electricity prices and redispatch costs*, 54th Hawaii International Conference on System Sciences, 2021.
- F. vom Scheidt, and P. Staudt, *Spatially Resolved Hydrogen Demand for Germany in 2030*, Mendeley Data, doi: 10.17632/8kyxj9khvv.1, 2021.
- F. vom Scheidt, C. Müller, P. Staudt, C. Weinhardt, *The German Electricity System in 2030: Data on Consumption, Generation, and the Grid*, Repository KITopen, doi: 10.5445/IR/1000125576, 2020.

Nomenclature

Sets and indices

C	Set of consumption locations c
D	Set of all days d in a year
$P = P_{Production} \bigcup P_{Import}$	Set of domestic production locations and import locations p
$S \in \{LH2, GH2, LOHC\}$	Set of hydrogen transportation states s

Decision variables

$X_p \in \{0,1\}$	Hydrogen production/import at location p (1), or not (0)
$HP_p \in [0,\infty)$	Daily amount of hydrogen production at p [kg_{H_2}/day]
$Y_{p,c} \in \{0,1\}$	Hydrogen transport from p to c (1), or not (0)
$HT_{p,c} \in [0,\infty)$	Daily amount of hydrogen transportation from p to c [kg_{H_2}/day]

Objective function parameters

PCC_p	Annual production capital cost at p [EUR]
POC_p	Annual production operating cost at p [EUR]
$CCC_{p,s}$	Annual conversion capital cost of s at p [EUR]
$COC_{p,s}$	Annual conversion operating cost of s at p [EUR]
TCC_s	Annual transportation capital cost of s [EUR]
TOC_s	Annual transportation operating cost of s [EUR]
SCC_s	Annual fueling station capital cost of s [EUR]
SOC_s	Annual fueling station operating cost of s [EUR]

Exogenous parameters

a	Depreciation period [years]
AF	Annuity factor [%]
CAP_{Import}	Import capacity [kg_{H_2}/day]

$CAP_{Production,max}$	Maximum production capacity [kg_{H_2}/day]
$CAP_{Production,min}$	Minimum production capacity [kg_{H_2}/day]
$CAP_{Trailer_s}$	Capacity of delivery trailer for state s [kg_{H_2}]
$DIST_{p,c}$	Air-line distance between p and c [km]
DF	Detour factor [-]
DS	Driving speed [km/h]
DT_s	Sum of driving time of delivery trucks [hours]
EC	Electricity consumption [kWh_{el}/kg_{H_2}]
ED	Energy density of hydrogen [kWh_{H_2}/kg_{H_2}]
EE	Electric efficiency of electrolysis [kWh_{H_2}/kWh_{el}]
EP	Uniform single electricity price [EUR/kWh_{el}]
EP_p	Electricity price at p [EUR/kWh_{el}]
FC	Fuel consumption of delivery truck [$liter/km$]
$FLH_{Electrolyzer}$	Full load hours of electrolyzers [hours]
FP	Fuel price [EUR/kg_{H_2}]
FSC	Fuel station capacity [kg/day]
FTC	Fuel and toll costs [EUR]
NGC_s	Natural gas consumption of fuel station of hydrogen state s [kWh_{NG}/kg_{H_2}]
HD_c	Daily hydrogen demand at location c [kg_{H_2}/day]
HIC	Hydrogen import costs [EUR/kg_{H_2}]
$IC_{Conversion_s}$	Investment costs of conversion equipment [EUR]
$IC_{Electrolyzer}$	Capacity-dependent investment costs of electrolyzer [EUR/kW_{el}]
$IC_{Station_s}$	Investment cost per fuel station for state s [EUR]
$IC_{Trailers_s}$	Investment cost per trailer for state s [EUR]
IC_{Trucks}	Investment cost per truck [EUR]
IS_s	Investment cost per fuel station of state s [EUR]
LC	Labor costs [EUR]
LT_s	Duration of loading and unloading one delivery trailer of state s [hours]
NS	Number of fuel stations [-]
NGP	Natural gas price [EUR/kWh_{NG}]

NT_s	Number of trucks for state s [-]
$O\&M$	Operation and maintenance cost factor [%]
T	Toll [EUR/km]
W	Wage [EUR/$hour$]
$WACC$	Weighted average cost of capital [%]

9.1 Introduction

Hydrogen produced from low-carbon sources can contribute substantially to mitigating emissions in sectors that are difficult or impossible to electrify directly. Governments worldwide and in particular in Europe, have announced strategies and billions of public funding to develop large-scale hydrogen infrastructure that is centered on electrolytic hydrogen supply (Hydrogen Council and McKinsey & Company, 2021). Since hydrogen production from electrolysis uses large amounts of electricity, a future hydrogen sector will introduce new interdependencies with the electricity sector. While electricity prices influence the cost-minimal installation (vom Scheidt et al., 2021) and operation (Guerra et al., 2019) of electrolyzers, these electrolyzers in turn introduce new electricity demand into the power system, influencing in the short term the usage of renewable energy (Ruhnau, 2020; Bødal et al., 2020) as well as congestion of power grids (vom Scheidt et al., 2021; Xiong et al., 2021) and in the long term the need for electricity generation and transmission capacity (Bødal et al., 2020). Most importantly, the effects of these interdependencies will be strong and will prevail for a long time, because electrolyzers are large-scale, stationary consumers with typical lifetimes of ten years and more (Schmidt et al., 2017).

The integration of electrolyzers in European grids raises some unique questions as European wholesale power markets are designed as single-price zonal markets that overlook intra-zonal transmission capacities and nodal price variations. Such single-price zonal market designs are already leading to rising congestion management costs in many electricity systems (Staudt et al., 2017). In Germany, the costs for congestion management have risen to around a billion Euro annually, and especially the curtailment of renewable energy plants is increasing (Xiong et al., 2021). Yet, political decision makers have repeatedly proclaimed that nodal pricing will not be introduced in Germany or Europe, any time soon (CDU, CSU und SPD, 2018; European Network of Transmission System Operators for Electricity, 2021). Without appropriate policy to guide system-beneficial integration, hydrogen production might strongly aggravate these effects. While the importance of market cost-reflective price regulation and subsidization of electrolyzers has been voiced in the political sphere (European Commission, 2020), there is a prevailing lack of energy policy research to guide efficient integration of hydrogen infrastructure into the electricity sector.

Therefore, in this chapter, we link an electrolytic hydrogen supply chain model with an electricity system dispatch model to analyze the cost-minimal hydrogen infrastructure setup under different electricity price signals, using Germany as a case study. We find that under current regulation with uniform single electricity prices, the cost-minimal solution is to produce hydrogen close to locations of consumption. These locations partly coincide with high locational marginal electricity costs. Consequently, our results also show how hydrogen production aggravates the inefficiencies of single-price markets and how it increases congestion management costs substantially, by increasing the need for redispatch.

We compare this benchmark scenario to a case in which electrolyzers are offered dedicated nodal tariffs, based on the Locational Marginal Prices that would form in a nodal pricing system. We find that such nodal signals lead to higher shares of hydrogen production at low-price nodes, longer transport distances, and lower total costs for hydrogen. This demonstrates the sensitivity of hydrogen supply chains to spatial prices or subsidies. Moreover, in this scenario, the integration of hydrogen leads to congestion management costs that are substantially lower than in the benchmark scenario and even below the baseline scenario without hydrogen. Interestingly, these avoided redispatch costs could effectively cover the subsidies a regulator would have to pay to mimic nodal prices for hydrogen electrolysis within the existing single-price zonal market design. Moreover, the system-wide CO_2 emissions decrease in the nodal tariff scenario, as electrolyzers are placed closer to renewable generation capacity.

Thus, in a time in which many policy makers and regulators in single-price zonal markets are planning future hydrogen supply systems, electricity tariff designs for electrolyzers, and subsidies for hydrogen infrastructure, our study demonstrates and quantifies the considerable benefits of differentiating these economic signals with respect to spatial criteria.

9.2 Background

Several past studies address the spatial aspects of hydrogen supply chains that use grid electricity for hydrogen production. Robinius et al. (2017), Reuß et al. (2019), and Emonts et al. (2019) present related models that link a hydrogen supply chain with a national electricity grid. The authors apply their model to the case of hydrogen fueled passenger cars in Germany in 2050 and identify favorable regions for hydrogen production in Germany. The studies do not explicitly consider effects of (spatial) economic signals, but rather take a technical supply chain perspective. Runge et al. (2019) optimize supply chains for synthetic fuels, including hydrogen stored in liquid organic hydrogen carrier (LOHC) material. Besides considering uniform single-prices, the authors also present a case in which they calculate state-level representative nodal prices for two exemplary states in Germany (NUTS-2 level) and allow transportation of hydrogen between the two states. This causes increased hydrogen production in the state with lower prices. The authors acknowledge the importance of future work analyzing feedback effects on the electricity system. Addressing this identified research gap is one of the contributions of our study.

Zhang et al. (2020a) analyze the flexible operation of electrolyzers that produce hydrogen for light, medium- and heavy-duty fuel cell electric vehicles (FCEVs) in the Western United States of America. They find evidence that increasing electrolyzer flexibility lowers hydrogen and electricity generation costs and CO_2 emissions. With a similar focus on temporal aspects, it has been demonstrated that flexibility of electrolytic hydrogen production enables more renewable integration for case studies in Texas, USA (Bødal et al., 2020), the Northeastern US (He et al., 2021) and Germany (Ruhnau, 2020).

Rose and Neumann (2020) focus on hydrogen supply for heavy-duty trucks from on-site electrolysis at highway fuel stations. They jointly optimize the infrastructure of fuel stations and the electricity system. They find that fully using hydrogen fueled heavy-duty trucks in Germany in 2050 would increase the total electricity demand by about 60 TWh and cause additional infrastructure costs of about 12 billion Euro per year. They note that nodal prices contain important information about "cost-effective energy consumption from a system perspective" and that investors in hydrogen infrastructure should consider the system perspective. This idea is expanded and implemented by vom Scheidt et al. (2021). The authors link a hydrogen supply chain optimization model and a nodal electricity system dispatch model and observe their interdependence in an initial case study of hydrogen-fueled trucks and passenger cars. They find that compared to current zonal uniform prices, nodal prices would lead to more hydrogen generation at low-price nodes. This in turn causes substantially lower congestion management costs. However, their analysis, like all previous ones, focuses on a small subset of hydrogen demand, i.e. demand from the transport sector.

Xiong et al. (2021) provide another perspective on the topic of hydrogen integration in single-price electricity markets. They do not consider the effects of hydrogen production on day-ahead energy wholesale markets, but analyze how Power-to-Gas plants (e.g. electrolyzers) can serve as a redispatch option. They find that curtailment of renewable generation can be reduced by 12% when electrolyzers are installed for performing redispatch at a few frequently curtailed nodes in the German grid of 2015. The study thus showcases the importance of spatial consideration in hydrogen infrastructure planning. However, the study ignores spatial aspects of the hydrogen supply chain and disregards how policy makers could incentivize investors to build electrolyzers at the identified nodes. Moreover, the direct political applicability of the study is restricted, because future hydrogen volumes, shares of renewable and conventional generation, and spatial distribution of generation will be very different than in the used scenario from 2015.

In summary, past research indicates that the spatial dimension of hydrogen integration matters. Within the limitations of single sector analyses or a reduced network consideration, studies have demonstrated that electrolyzer locations influence grid congestion. However, to the best of our knowledge, no past study has evaluated the cost-optimal hydrogen supply chain for electrolytic hydrogen for a broad range of hydrogen demand sectors, namely steel, ammonia, methanol, refineries, and transportation, considered the effect of alternative electricity price signals, and assessed the feedback effects of the resulting supply chains on the electricity system. Such an analysis is timely from a policy perspective, given the prospect of significant electrolyzer capacity integration over the next decade in the German and European power grid.

9.3 Methods

To address this topic, we model the hydrogen supply chain and the electricity system and link both models through their respective inputs and outputs. As shown in Figure 9.1, we proceed in three steps. First, we parametrize an electricity system dispatch model without hydrogen and compute uniform prices, nodal prices, redispatch costs, and CO_2 emissions. Second, utilizing the computed electricity prices, we run the hydrogen model to identify the cost-minimal spatial siting of electrolyzers, their capacities, and the form of hydrogen transportation.[24] We consider a scenario with uniform zonal prices to reflect current regulation and a scenario with nodal prices to reflect a more efficient solution. For both scenarios, we calculate a case of static electrolyzer operation and a case of dynamic, i.e. flexible operation. Third, we feed back the resulting locations and capacities of the electrolyzers as additional regional loads into the electricity model. We calculate consequential changes in wholesale electricity prices and congestion management costs. Both models are implemented in Python 3.7.3, and solved using the Gurobi solver 8.1.1.

9.3.1 Hydrogen supply chain model

In the following, we describe the details of the hydrogen supply chain model. It represents an enhanced version of the model in vom Scheidt et al. (2021). Due to the temporal uncertainty in demand from end-use sectors, the model assumes time-invariant hydrogen consumption.

[24]Note that we neglect non-energy components of tariffs, such as grid charges, taxes and other charges, because they are assumed to not affect the placing and operation of electrolyzers. Therefore, we assume that the calculated electricity prices equal the final tariff paid by the electrolyzer operator.

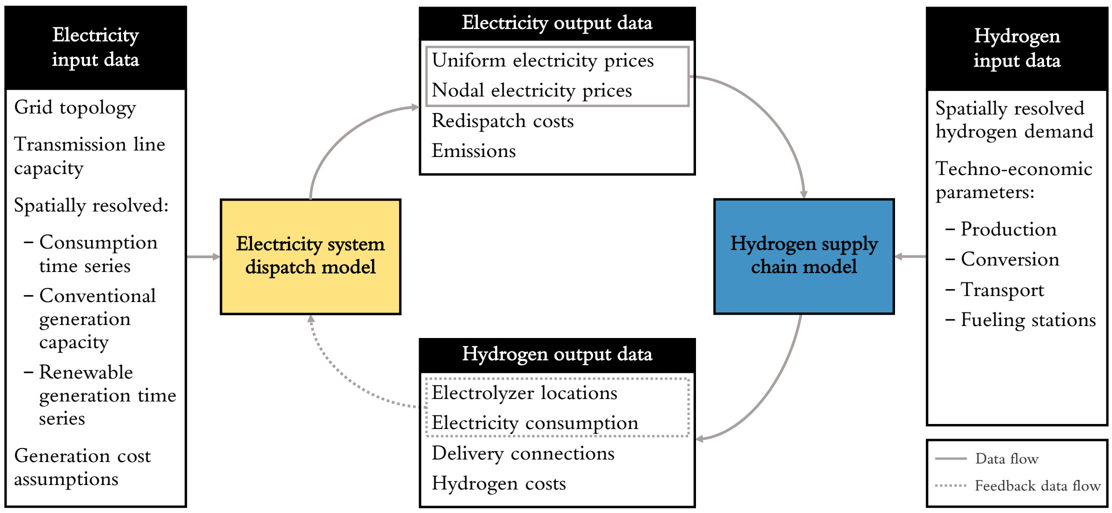


Figure 9.1.: Method overview: Models for the hydrogen and the electricity system, linked through inputs and outputs

Objective function

The model minimizes the total annual end-use costs of hydrogen, which consist of capital costs and operating costs for electrolytic production (PCC, POC), conversion (CCC, COC) and transportation (TCC, TOC) of hydrogen, and, in the case of hydrogen use in the transportation sector, the fueling stations (SCC, SOC) (Equation 9.1). For this, the model optimizes the location and size of electrolyzers and the amount of hydrogen that is transported from each electrolyzer to each location of consumption. There are four decision variables. (i) X_p is a binary variable that indicates whether an electrolyzer is installed at a location p (1) or not (0). (ii) $HP_p \in [0, \infty)$ denotes the amount of hydrogen produced at p in kg_{H_2} per day. (iii) $Y_{p,c}$ is binary and indicates whether hydrogen is transported from a production location p to a consumption location c (1) or not (0). (iv) $HT_{p,c} \in [0, \infty)$ denotes the amount of hydrogen transported from p to c in kg_{H_2} per day. P and C represent the set of all potential electrolyzer plant locations p, and consumption locations c, respectively. Thus, the model outputs the cost-minimal locations of electrolyzers, their individual daily production, the transportation volume between each electrolyzer and point of consumption, and the resulting end-use costs of hydrogen.

$$\begin{aligned}\min_{X_p, HP_p, Y_{p,c}} (\sum_{p \in P} PCC_p(\boldsymbol{X_p}, \boldsymbol{HP_p}) + \sum_{p \in P} \sum_{d \in D} POC_p(\boldsymbol{X_p}, \boldsymbol{HP_p}) \\ + \sum_{p \in P} CCC_{p,s} + \sum_{p \in P} COC_{p,s}(\boldsymbol{X_p}, \boldsymbol{HP_p}) \\ + TCC_s + \sum_{p \in P} \sum_{c \in C} TOC_{p,c,s}(\boldsymbol{Y_{p,c}}, \boldsymbol{HT_{p,c}}) \\ + SCC_s + SOC_s)\end{aligned} \tag{9.1}$$

The model can be parametrized for three possible hydrogen states s of transportation via delivery trailers: liquefied (LH2), compressed gaseous (GH2), and bound in LOHC. These three states require different technologies for conversion, transportation and fueling stations and thus cause different costs. The annotation of decision variables, indices and input variables is provided in the nomenclature.

The four components of capital costs include specific annual operation and management costs ($O\&M$) and annuity factors (AF). The annuity factors account for the depreciation of one-time investments over multiple years and depend on the weighted average cost of capital ($WACC$ [%]) and depreciation periods (a [years]) (Eq. 9.2).

$$AF = \frac{(1 + WACC)^a \cdot WACC}{(1 + WACC)^a - 1} \tag{9.2}$$

Production capital costs occur at a location only if an electrolyzer is placed there, and depend on the daily hydrogen output capacity (Eq. 9.3).

$$\begin{aligned}PCC_p = \boldsymbol{X_p} \cdot \frac{\boldsymbol{HP_p} \cdot ED \cdot IC_{Electrolyzer}}{FLH \cdot EE} \cdot (1 + O\&M_{Electrolyzer}) \\ \cdot AF_{Electrolyzer} \ \ \forall p \in P_{Production}\end{aligned} \tag{9.3}$$

Production operating costs depend on the amount of hydrogen that is produced, the efficiency of the electrolyzer, and the electricity price EP_p (Eq. 9.4). Note that this price varies with location p.

$$POC_p = \boldsymbol{HP_p} \cdot EC_{Production} \cdot EP_p \cdot 365 \ \ \forall p \in P_{Production} \tag{9.4}$$

In addition to domestic hydrogen production, the model also includes overseas imports. Imports do not incur any capital costs for production (Eq. 9.5), but specific production operating costs (Eq. 9.6).

$$PCC_{Import} = 0 \tag{9.5}$$

$$POC_{Import} = HP_{Import} \cdot HIC \cdot 365 \tag{9.6}$$

Moreover, conversion capital costs are assumed to occur in bulk (depending on the total amount of hydrogen that needs to be converted daily) and independently of the location (Eq. 9.7). They do, however, depend on the state in which hydrogen is to be transported afterwards, namely gaseous, liquefied, or stored in LOHC.

$$CCC_s = IC_{Conversion_s} \cdot (1 + O\&M_{Conversion_s}) \cdot AF_{Conversion_s} \;\; \forall s \in S \tag{9.7}$$

Furthermore, the model includes the operating costs of converting hydrogen. For liquid delivery, hydrogen needs to be liquefied and later evaporated at the location of consumption, which requires electricity (Eq. 9.8).

$$\begin{aligned} COC_{p,LH2} = (&\sum_{p \in P_{Production}} \boldsymbol{HP_p} \cdot EC_{Liquefaction} \cdot EP_p \cdot (1 + Loss_{Liquefaction})) \\ &+ (\sum_{p \in P} \boldsymbol{HP_p} \cdot EC_{Evaporation} \cdot EP \cdot (1 + Loss_{Evaporation})) \cdot 365 \end{aligned} \tag{9.8}$$

In the case of gaseous delivery, hydrogen is compressed as specified in (Eq. 9.9).

$$COC_{p,GH2} = \sum_{p \in P_{Production}} \boldsymbol{HP_p} \cdot EC_{Compression} \cdot EP_p \cdot (1 + Loss_{Compression}) \cdot 365 \tag{9.9}$$

For LOHC delivery, the carrier material needs to be hydrogenated and later dehydrogenated at the location of consumption (Eq. 9.10). Electricity is required for both steps. Additionaly, natural gas is required for dehydrogenation.

$$\begin{aligned} COC_{p,LOHC} = (&\sum_{p \in P \setminus Import} \boldsymbol{HP_p} \cdot EC_{Hydrogenation} \cdot EP_p \cdot (1 + Loss_{Hydrogenation})) \\ &+ (\sum_{p \in P} \boldsymbol{HP_p} \cdot (EP \cdot EC_{Dehydrogenation} + NGP \cdot NGC_{Dehydrogenation}) \\ &\cdot (1 + Loss_{Dehydrogenation})) \cdot 365 \end{aligned} \tag{9.10}$$

For LH2 and LOHC, we assume that imports already arrive in the respective form and thus do not require the first conversion step for domestic delivery. After initial conversion, hydrogen is transported to the consumption sinks. In general, hydrogen can be transported via tube trailers mounted onto delivery trucks or via pipelines. Since related work indicates that transport via pipelines only becomes economically viable for long transport distances in high demand scenarios (Reuß et al., 2019; Robinius et al., 2017; Tlili et al., 2020), our model focuses on transport via tube trailers on delivery trucks.[25] Thus, transport capital costs depend on the investment costs for hydrogen trailers and the respective transport trucks, as well as the number of trailers and trucks. Each truck carries one trailer.

$$\begin{aligned} TCC_s = IC_{Trucks} \cdot NT_s \cdot (1 + O\&M_{Trucks}) \cdot AF_{Trucks} + IC_{Trailers_s} \cdot NT_s \\ \cdot (1 + O\&M_{Trailers_s}) \cdot AF_{Trailers} \quad \forall s \in S \end{aligned} \tag{9.11}$$

Transport operating costs consist of costs for labor LC as well as fuel and toll FTC (Eq. 9.12).

$$TOC_s = (LC + FTC) \cdot 365 \tag{9.12}$$

Daily labor costs depend on the drivers' wage W, and the time that drivers spend loading and unloading (LT_s) as well as driving (DT_s) the delivery trailers (Eq. 9.13).

[25]Future work could expand our model by including both truck based and pipeline based hydrogen transportation. This could lead to lower end-use hydrogen costs. However, it would likely not affect this study's findings regarding optimal electrolyzer locations and redispatch in a substantial manner, because hydrogen transportation costs have a much smaller impact on total costs and thus optimal locations than hydrogen production costs (compare 9.6). Therefore, even if transportation costs were lower in a pipeline scenario, this would not lead to different results regarding the cost-optimal location of electrolyzers, redispatch, and emissions.

A fixed loading and unloading time per delivery is assumed.

$$LC = (DT_s + LT_s \cdot NT_s) \cdot W \tag{9.13}$$

Daily round-trip driving time is determined by the distance between connected production plants and points of consumption ($DIST_{p,c}$) as well as the driving speed DS. Transport distances are approximated via air-line distance, multiplied with a detour factor DF of 1.3, in line with Reuß (2019). Since the daily capacity of fueling stations is assumed to be smaller than the capacity of one delivery trailer, we multiply the distances to fueling stations with a frequency factor $HD_c/CAP_{Trailer_s}$ (Eq. 9.14) simulating that they are not provided with hydrogen on a daily basis. This also applies to daily fuel and toll costs (Eq. 9.15).

$$\begin{aligned} DT_s = \frac{2 \cdot DF}{DS} \cdot (&\sum_{p \in P} \sum_{c \in C_{Industry}} \boldsymbol{Y_{p,c}} \cdot DISTp,c \\ &+ \sum_{p \in P} \sum_{c \in C_{Stations}} \boldsymbol{Y_{p,c}} \cdot DIST_{p,c} \cdot \frac{HD_c}{CAP_{Trailer_s}}) \end{aligned} \tag{9.14}$$

$$\begin{aligned} FTC = 2 \cdot (FC_{Truck} \cdot FP + T) \cdot DF \cdot ((&\sum_{p \in P} \sum_{c \in C_{Industry}} \boldsymbol{Y_{p,c}} \cdot DISTp,c) \\ &+ (\sum_{p \in P} \sum_{c \in C_{Stations}} \boldsymbol{Y_{p,c}} \cdot DIST_{p,c} \cdot \frac{HD_c}{CAP_{Trailer_s}})) \end{aligned} \tag{9.15}$$

For hydrogen that is to be used to refuel fuel cell trucks or passenger cars, one additional supply chain step is modelled: the fuel station. The capital costs for fuel stations depend on the investment costs per station and the total number of stations (Eq. 9.16).

$$SCC_s = IC_{Station_s} \cdot NS \cdot (1 + O\&M_{Station}) \cdot AF_{Station} \quad \forall s \in S \tag{9.16}$$

The operating costs depend on the required consumption of electricity and natural gas and their respective prices (Eq. 9.17).

$$\begin{aligned} SOC_s = (&EC_{Station_s} \cdot EP + NGC_{Station_s} \cdot NGP) \\ &\cdot (1 + Loss_{Station_s}) \cdot \sum_{c \in C_{Stations}} HD_c \cdot 365 \end{aligned} \tag{9.17}$$

Constraints

The model includes both domestic production and an exogenously given import at one fixed node. The sum of daily domestic and imported hydrogen production HP must satisfy the sum of the exogenously given daily demand HD (Eq. 9.18). The model assumes a constant daily demand at each node.

$$\sum_{p \in P} \boldsymbol{HP_p} = \sum_{c \in C} HD_c \tag{9.18}$$

Daily hydrogen output HP_p of each electrolyzer is limited by its maximum and minimum daily production capacity (Eq. 9.19 and Eq. 9.20).

$$\boldsymbol{HP_p} \geq CAP_{Production,min} \cdot \boldsymbol{X_p} \;\; \forall p \in P_{Production} \tag{9.19}$$

$$\boldsymbol{HP_p} \leq CAP_{Production,max} \cdot \boldsymbol{X_p} \;\; \forall p \in P_{Production} \tag{9.20}$$

The import nodes and their capacity are exogenously set in Eq. 9.21 and 9.22.

$$\boldsymbol{X_p} = 1 \;\; \forall p \in P_{Import} \tag{9.21}$$

$$\boldsymbol{HP_p} = CAP_{Import} \cdot \boldsymbol{X_p} \;\; \forall p \in P_{Import} \tag{9.22}$$

In sum, the daily amount of hydrogen transported from a hydrogen source (electrolyzer or import) must not exceed the available hydrogen at that node (Eq. 9.23).

$$\sum_{c \in C} \boldsymbol{HT_{p,c}} \leq \boldsymbol{HP_p} \;\; \forall p \in P \tag{9.23}$$

The daily amount transported to a consumer must meet its daily demand (Eq. 9.24).

$$\sum_{p \in P} \boldsymbol{HT_{p,c}} \geq HD_c \;\; \forall c \in C \tag{9.24}$$

Positive transport volume from a plant p to a consumption location c is only possible if the delivery connection is established via the binary variable $Y_{p,c}$ (Eq.

9.25).

$$\begin{aligned} \boldsymbol{HT_{p,c}} &= 0, if \ \ \boldsymbol{Y_{p,c}} = 0 \ \ \forall c \in C, \forall p \in P \\ \boldsymbol{HT_{p,c}} &> 0, if \ \ \boldsymbol{Y_{p,c}} = 1 \ \ \forall c \in C, \forall p \in P \end{aligned} \tag{9.25}$$

Thus, one limitation of the model is that it does not consider short term or long term temporal variations in hydrogen transportation or consumption and thus neglects storage. While out of scope of this study, future work could attempt to identify short term and long term temporal patterns of hydrogen demand from industry and transportation.[26] We do assess a sensitivity case in which transportation and consumption remain continuous, but the production is temporally flexible and can exploit low electricity prices in certain hours. This allows us to identify an optimistic estimate of the potential cost savings that flexible electrolyzer operation can yield.

9.3.2 Electricity system model

Next, we model the electricity system to calculate electricity prices, redispatch costs, and emissions.

For the uniform price scenario, we adapt a stylized merit-order and redispatch model from Staudt and Oren (2020). For each hour, the model minimizes the marginal generation costs for the entire single-price market zone (Eq. 9.26). The model's constraints ensure that demand and supply are balanced (Eq. 9.27) subject to the constraints that limit available generation capacity (Eq. 9.28). The annotation for the electricity system model is given in Table 9.2.

$$\min \left(\sum_{t=1}^{T} \sum_{n=1}^{N} \sum_{g=1}^{G} q_{n,g,t} \cdot p_{n,g}\right) \tag{9.26}$$

$$s.t. \sum_{n=1}^{N} d_{n,t} = \sum_{n=1}^{N} \sum_{g=1}^{G} q_{n,g,t} \ \ \forall t \in T \tag{9.27}$$

$$q_{n,g,t} \leq c_{n,g,t} \ \ \forall g \in G, \ \ \forall n \in N, \ \ \forall t \in T \tag{9.28}$$

[26]Regarding long term storage, techno-economic parameters are presented by Reuß et al. (2019) and locations with high geological potential for hydrogen storage are presented by Caglayan et al. (2020).

Complying with the market designs of single-price markets, this model does not consider grid constraints. Therefore, the resulting market allocation can be technically infeasible, in which case redispatch measures ensue, modelled by Eq. 9.29 to 9.33. The cost based redispatch mechanism begins with the existing market allocation and activates and deactivates generation capacity in the system until the cost-minimal solution is found that respects grid constraints, which in the optimal case is equivalent to the nodal pricing solution (Staudt, 2019). Generators that are activated through this procedure are compensated based on their operating costs. The additional costs caused by this procedure are referred to as redispatch costs. In the considered idealized case, they are equivalent to the congestion management costs.

$$\min\,(\sum_{n=1}^{N}\sum_{g=1}^{G} q^{\Delta}_{n,g,t} \cdot p_{n,g}) \;\; \forall t \in T \tag{9.29}$$

$$s.t. \sum_{n=1}^{N}\sum_{g=1}^{G} q^{\Delta}_{n,g,t} = 0 \;\; \forall t \in T \tag{9.30}$$

$$q^{\Delta}_{n,g,t} + q_{n,g,t} \leq c_{n,g,t} \;\; \forall n \in N, \;\; \forall g \in G, \;\; \forall t \in T \tag{9.31}$$

$$q^{\Delta}_{n,g,t} + q_{n,g,t} \geq 0 \;\; \forall n \in N, \;\; \forall g \in G, \;\; \forall t \in T \tag{9.32}$$

$$|\sum_{n=1}^{N}\sum_{g=1}^{G} (((q_{n,g,t} + q^{\Delta}_{n,g,t}) - d_{n,t}) \cdot H_{l,n})| \;\; \leq \tau_l \forall l \in L, \;\; \forall t \in T \tag{9.33}$$

For the nodal price scenario, we use a nodal model with a DC-load flow approximation. This model simultaneously takes into account generation capacities and costs (Eq. 9.26 to 9.28), as well as capacity constraints (Eq. 9.34).

$$|\sum_{n=1}^{N}\sum_{g=1}^{G} ((q_{n,g,t} - d_{n,t}) \cdot H_{l,n})| \leq \tau_l \;\; \forall l \in L, \;\; \forall t \in T \tag{9.34}$$

Both models optimize each hour step-wise, independently of other hours. They thus neglect generation ramping and storage. Last, emissions are calculated based on the resulting electricity generation of the individual plants and their average emissions factor (vom Scheidt et al., 2020).

Table 9.2.: Notation for electricity system model

$q_{n,g,t}$	Generation of unit g at node n at time t
$q^{\Delta}_{n,g,t}$	Redispatch of unit g at node n at time t
$p_{n,g}$	Marginal generation costs of unit g at node n
$d_{n,t}$	Demand at node n at time t
$c_{n,g,t}$	Generation capacity of unit g at node n (at time t for renewables)
τ_l	Transmission capacity of line l
H	Matrix of power distribution factors
N	Number of nodes n
G	Number of generation units g
L	Number of lines l

9.4 Case study

To demonstrate the functioning of the hydrogen model and the electricity model, we apply it to a case study. For this, we parametrize the models with data for the German electricity system and hydrogen demand in 2030.

9.4.1 Hydrogen data

In this subsection, we present all data sources, preprocessing steps, and assumptions used for creating the input data sets for demand, production, conversion, and transportation of hydrogen.

Hydrogen demand

In the following paragraphs, we describe data acquisition and preprocessing for the German hydrogen net demand in 2030. Hydrogen demand is assumed to come from the six following sectors: steel, ammonia, methanol, refinery, road transportation, and individual mobility. First, each demand sector is presented with general assumptions about future hydrogen demand and potential. Subsequently, the relevant locations and volumes of hydrogen demand in the respective sector in 2030 are identified. Table A.1 in Appendix F shows the numeric values and conversion factors used for the hydrogen demand calculations. For steel, ammonia, methanol, and refineries, 100% availability of the production facilities is assumed. Correspondingly, quantities that have been calculated down to hours are multiplied by 8,760 to get

Table 9.3.: Estimated hydrogen demand of ammonia producers in Germany, 2030

Ammonia producer	Hydrogen net demand [TWh]
BASF Ludwigshafen	5.18
INEOS Köln	2.25
SKW Stickstoffwerke Piesteritz	5.62
YARA Brunsbüttel	4.44
Total	17.49

the respective annual quantity. For details on data acquisition and processing, we refer to Appendix E. All data is available at vom Scheidt and Staudt (2021).

Ammonia. Ammonia (NH_3) is produced using the Haber-Bosch process and requires the input components hydrogen (H_2) and nitrogen (N_2) (Hermann et al., 2014). The potential for CO_2 emissions reduction lies in replacing fossil fuel based hydrogen with electricity based hydrogen. Today, hydrogen is mostly produced from steam methane reforming, with the by-product CO_2. This byproduct can be used for processes in material composites, such as the production of urea (Hebling et al., 2019). Nevertheless, our estimation assumes a complete switch of ammonia production to electricity based hydrogen in order to define an upper limit of hydrogen demand in the ammonia industry. Table 9.3 summarises the hydrogen demand from electrolysis of the ammonia industry. Based on the assumptions made, the total hydrogen demand is 17.49 TWh, distributed over four plants.

Steel. Steel production in Germany offers a large potential for the use of hydrogen in industry by switching to hydrogen based processes. In general, a distinction is made in steel production between primary and secondary steel as well as between blast furnace and electric arc routes (Hebling et al., 2019). Today, primary steel production is mainly based on coal- or coke based processes to reduce iron ore in the blast furnace, resulting in large amounts of carbon emissions (Wilms et al., 2018). An alternative to the blast furnace is direct reduction, in which the iron ore is reduced by natural gas or hydrogen, avoiding CO_2 emissions (Hebling et al., 2019). The directly reduced iron is further processed into steel in an electric arc furnace. If hydrogen is produced by electrolysis with electricity from renewable energy and used instead of coal in the direct reduction process, up to 95% of CO_2 emissions could be avoided on the way to primary steel (Berger, 2020). In addition to the possibility of

Table 9.4.: Estimated hydrogen net demand of primary steel producers in Germany, 2030

Steel producer	**Hydrogen net demand [TWh]**
ArcelorMittal Bremen	0.0
ArcelorMittal Duisburg	0.0
ArcelorMittal Eisenhüttenstadt	0.0
ArcelorMittal Hamburg	2.67
ROGESA (Dillinger & Saarstahl)	2.16
HKM Duisburg	0.0
Salzgitter Peine	2.25
Thyssenkrupp Steel Europe Duisburg	6.17
Total	13.25

switching to direct reduction, CO_2 emission reductions can be achieved by blowing in hydrogen as a substitute reducing agent. The basic idea is to reduce the amount of injection coal required and to replace it with hydrogen, in order to reduce CO_2 emissions (Thyssenkrupp, 2019). Depending on the operating conditions, emissions can be reduced by 21.4 - 28.5 % compared to a reference case with today's standard operating mode (Yilmaz, 2018).

We identify all steel plants with potential for hydrogen use in 2030 through an extensive review of industry reports and press releases, as elaborated in Appendix A. Table 9.4 summarizes the hydrogen net demand of the steel industry. Based on the assumptions made, the total hydrogen net demand for 2030 amounts to 13.25 TWh and is distributed over Hamburg, Dillingen/Saar, Peine and Duisburg.

Methanol. Currently, methanol is commonly produced using synthesis processes with CO_2 emissions, which, in the future, can be switched to hydrogen based processes (Michalski et al., 2019). Table 9.5 summarises the hydrogen demand of the methanol industry. Based on the assumptions made, the total hydrogen demand is 11.73 TWh and is distributed over four sites.

Refineries. In refineries, hydrogen is used on a large scale to desulfurize fuels and to refine heavy residues with hydrogen via hydrocracking (Hermann et al., 2014). The hydrogen needed for crude oil processing is supplied from internal and external sources. This means that refineries are partly self-sufficient, since hydrogen is a by-product of other processing operations (ENCON.Europe GmbH, 2018). In this study, a 22 % net demand for hydrogen is assumed, analogous to Wilms et al. (2018). This

Table 9.5.: Estimated hydrogen net demand of methanol producers in Germany, 2030

Methanol producer	Hydrogen net demand [TWh]
BASF Ludwigshafen	2.83
Shell Rheinland Raffinerie - Süd	2.74
Ruhr Oel - BP Gelsenkirchen	1.76
Total Raffinerie Mitteldeutschland	4.40
Total	11.73

Table 9.6.: Estimated hydrogen net demand of refineries in Germany, 2030

Refinery	Hydrogen net demand [TWh]
Bayernoil Raffineriegesellschaft	0.19
BP Raffinerie Lingen	0.21
Gunvor Raffinerie Ingolstadt	0.22
Holborn Europa Raffinerie	0.23
MiRO Mineraloelraffinerie Oberrhein	0.66
Nynas	0.08
OMV Deutschland	0.16
PCK Raffinerie	0.51
Raffinerie Heide	0.19
Ruhr Oel - BP Gelsenkirchen	0.57
Shell Rheinland Raffinerie Werk Nord	0.41
Shell Rheinland Raffinerie Werk Süd	0.32
Total Raffinerie Mitteldeutschland	0.53
Total	4.29

hydrogen net demand is assumed to be entirely served by electricity based hydrogen in 2030, in line with Prognos AG (2020b). Table 9.6 summarises the hydrogen net demand of the refineries in Germany 2030. The estimated total hydrogen net demand is 4.29 TWh and is distributed over thirteen sites in Germany.

Transportation sector. In the first step, we estimate the total national hydrogen demand in the transport sector and the number of fueling stations required to satisfy the demand. For this, we calculate a main scenario with fuel cell trucks, and a sensitivity scenario with additional fuel cell passenger cars. In the second step, we spatially disaggregate this total demand and determine potential sites for fueling stations.

Table 9.7.: Hydrogen fuel station assumptions

	LH2	GH2	LOHC
α $[-]$	0.6	0.7	0.66
β $[-]$	0.06	0.06	0.06
γ $[-]$	0.9	0.6	1.4
EC_s $[kWh_{el}/kg_{H_2}]$	0.6	1.6	4.4
NGC_s $[kWh_{NG}/kg_{H_2}]$	0	0	11.7
Depreciation years $[a]$	10	10	10
O&M [%]	5	5	5

To determine the hydrogen demand for fuel cell trucks and passenger cars in Germany in 2030, we use the mean estimates from Fraunhofer-Institut (2019), namely 1.00 TWh for trucks and 3.50 TWh for cars. For a sensitivity scenario without hydrogen demand for cars, see Appendix G. We assume that *heavy-duty* trucks with a total weight above 12,000 kg (European Alternative Fuels Observatory, 2020) will be responsible for all truck based demand, because they have particularly high carbon emission savings potential and the fuel cell based version has stronger advantages compared to their battery based counterparts, i.e. heavier payloads, longer ranges, and shorter recharging times (Weger et al., 2020). We assume the consumption of trucks to decrease to 8 $kg_{H_2}/100km$ until 2030, and that of fuel cell passenger cars to decrease to 0.63 kg/100km, in line with Grube and Stolten (2018), FCH-JU (2017), and Hyundai (2020).[27] We assume that by 2030 all hydrogen stations will become L-size (International Energy Agency, 2015) with a capacity of 1,000 kg/day. According to Reuß et al. (2019), station investment cost is estimated considering scaling and learning effects, based on Equation (9.35). With NS, the total number of fuel stations determined in our model, a capacity of each fuel station of FSC = 1,000 kg/day, and the exogenous parameters α, β, and γ presented in Table 9.7, we derive the investment cost per station for each hydrogen transportation state s.

$$IS_s = 1.3 \cdot 600,000EUR \cdot \gamma \cdot (\frac{FSC}{212kg/day})^{\alpha} \cdot (1-\beta)^{\log_2(\frac{FSC \cdot NS}{212kg/day \cdot 400})} \tag{9.35}$$

Next, we identify the number and locations of fueling stations. Since passenger

[27]This translates to approximately 1.2 million fuel cell cars, and approximately 11,000 fuel cell trucks.

cars and trucks have different driving and refueling patterns, we separately select their fuel station locations.

For passenger cars, we assume a fuel station utilization of 70% and thus a turnover of 700 kg_{H_2} per day, in line with Reuß et al. (2019). This results in 412 fueling stations for cars. We then first disaggregate the total demand to the >400 German NUTS-2 regions proportionally to the NUTS-2 gross domestic product (GDP). Since no more granular GDP data exists, we further break down the hydrogen demand to the over 10,000 NUTS-3 regions in Germany proportionally to the population in that NUTS-3 region. As of October 2019, there are 72 hydrogen fueling stations in Germany (H2 MOBILITY, 2019). Since these will not suffice to satisfy demand in 2030, we assume that additional fueling stations will be installed at the same locations as existing gasoline stations. Therefore, we use the 11,285 gasoline stations from OpenStreetMap as further potential sites (OpenStreetMap Contributors, 2020). For each of these stations, we calculate the distance to the closest NUTS-3 region center. For each NUTS-3 region, we then select stations with the shortest distance to its center, until its demand is covered.

For trucks, Rose and Neumann (2020) determine optimal hydrogen fuel station locations along highways under consideration of traffic flow and capacity limits. From these locations, we adopt those with highest utilization rate, which leads to 97 stations. We assume all fuel stations have 1,000 kg/day capacity and have the same turnover. Thus, to meet the demand from fuel cell heavy-duty trucks, the turnover of each fuel station is 847.42 kg_{H_2} per day.

Summary of hydrogen demand. The total hydrogen net demand in 2030 is estimated to be 51.26 TWh. Figure 9.2 displays the hydrogen net demands of the individual sectors. The map in Figure 9.3 shows the geographic distribution of the hydrogen demand, with the size of the markers corresponding to demand volume. The corresponding final hydrogen demand data with volumes and locations is available in vom Scheidt and Staudt (2021)

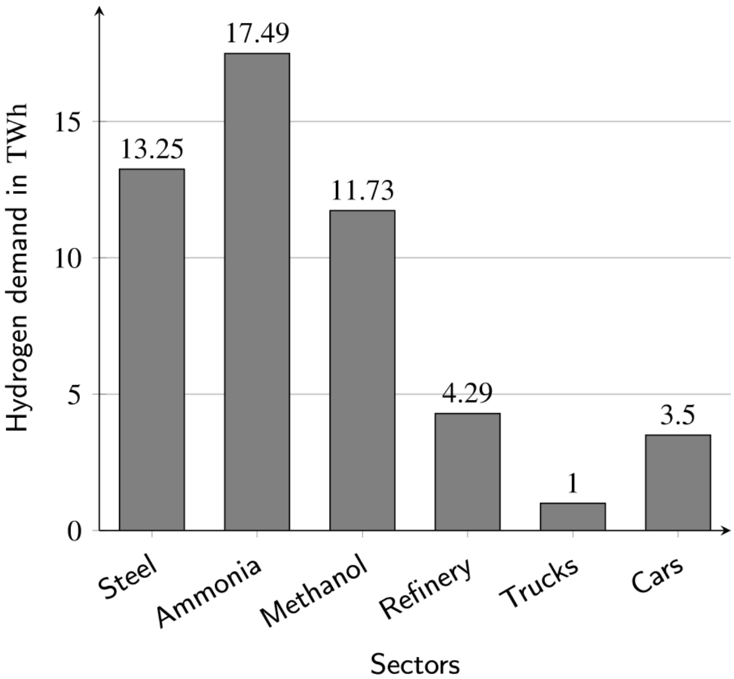


Figure 9.2.: Estimated hydrogen net demand per sector in Germany, 2030

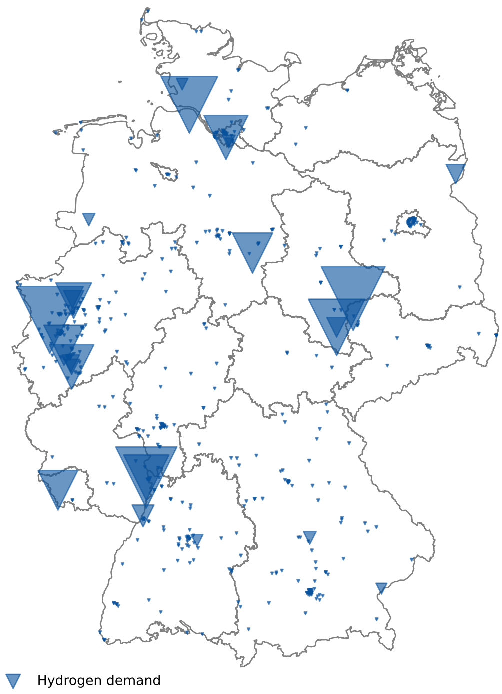


Figure 9.3.: Spatial distribution of estimated hydrogen net demand in Germany, 2030

Hydrogen production and import data

Electrolysis is the main pillar of political strategies for hydrogen supply in Germany (Bundesregierung, 2020) and the EU (European Commission, 2020). Among the different electrolysis technologies, proton exchange membrane (PEM) electrolysis is projected to have the lowest CAPEX and highest efficiency in 2030 (Böhm et al., 2020). Therefore, we focus on PEM electrolysis for hydrogen production. As input for the hydrogen supply chain model, we assume investment costs $IC_{Electrolyzer}$ of 604 EUR/kW_{el}, depreciation over 10 years, O&M costs of 4% of investment costs and electricity consumption EC of 47.6 kWh_{el} per kg_{H2} (Schmidt et al., 2017; Brown et al., 2018; Reuß et al., 2019). Electrolyzer efficiency EE is set to 70% (Heymann et al., 2021; Robinius et al., 2017; Reuß et al., 2019). We set the minimum capacity $CAP_{Production,min}$ to 10 MW and the maximum capacity $CAP_{Production,max}$ to 100 MW.[28] Regarding operation, we analyze two different cases. In the main case, all electrolyzers are assumed to operate continuously under a Flat tariff at 70% of full capacity, which is within typical ranges (Robinius et al., 2017; Guerra et al., 2019; Ruhnau, 2020). In a sensitivity case, all electrolyzers are assumed to operate under a real-time tariff and have temporal flexibility, which allows them to shift their operation to hours with cheap prices. In this case, we assume they run at 100% during the 70% cheapest hours. Thus, in both cases, the total volume of produced hydrogen is the same.

The potential locations for electrolyzers are equal to the set of transmission grid nodes from our electricity system model (compare Section 9.4.2).[29] Additionally, we include hydrogen imports from overseas into our model, since they are a key part of the German hydrogen strategy (Bundesregierung, 2020). For these imports, we assume a fixed, exogenous amount of daily available imported hydrogen of 27.40 GWh and costs of 3.48 EUR/kg_{H_2}, in line with the mean values reported by Runge et al. (2020). Furthermore, we assume that all imports to Germany will occur at one

[28]This range is determined based on a review of power-to-gas projects that are scheduled to be commissioned after 2021 in Germany (ELEMENT EINS, Energiepark Bad Lauchstädt, GET H2 Nukleus, HydroHub Fenne, GreenHydroChem Mitteldeutschland, Westküste100). All of them are in the range of 10-100 MW.

[29]Such large-scale electrolyzers might be complemented by smaller, on-site electrolyzers (see, e.g. Rose and Neumann (2020); Golla et al. (2020)) in practice. Such on-site electrolyzers would be connected to the distribution grid. Analyzing congestion consequences at distribution grid level is out of scope of this study.

Table 9.8.: Conversion assumptions, based on Reuß et al. (2019); Nexant et al. (2008). x denotes daily hydrogen output.

	Investment costs [EUR]	Depreciation years	O&M	$EC_{Conversion}$ $[kWh_{el}/kg_{H_2}]$	$NGC_{Conversion}$ $[kWh_{NG}/kg_{H_2}]$	Loss [%]
Compressor	$15 \cdot 10^3 \frac{EUR}{kW} \cdot x^{0.6089} \cdot 3$	15	4%	calculated	0	0.5
Liquefaction	$105 \cdot 10^6 EUR \cdot (\frac{x}{50 \frac{t_{H_2}}{day}})^{0.66}$	20	4%	6.78	0	1.65
Evaporation	$3 \cdot 10^3 EUR \cdot \frac{x}{1{,}000}$	10	3%	0.6	0	0
Hydrogenation	$40 \cdot 10^6 EUR \cdot (\frac{x}{300 \frac{t_{H_2}}{day}})^{0.66}$	20	3%	0.37	0	1
Dehydrogenation	$30 \cdot 10^6 EUR \cdot (\frac{x}{300 \frac{t_{H_2}}{day}})^{0.66}$	20	3%	0.37	11.7	1

large port, i.e. Bremerhaven, in line with Runge et al. (2020).

Hydrogen conversion data

Hydrogen can be converted to a liquefied state (LH2), compressed state (GH2), or stored into chemicals (LOHC) for transportation via tube trailers. Notably, for LH2 and LOHC, there are capital and operating costs at the point of hydrogen production (for liquefaction, and hydrogenation, respectively) and at the point of hydrogen consumption (evaporation, and dehydrogenation, respectively).

The assumptions regarding investment costs, depreciation years, O&M costs, electricity and natural gas consumption, and losses are displayed in Table 9.8.

Hydrogen transportation data

Transportation costs include costs for fuel, toll, and the drivers' wages. We assume that delivery trucks are fueled with hydrogen. The consumption is set to 5.19 kg_{H_2}/100km and the fuel price to 7.91 EUR/kg, including a value added tax of 19% (Fraunhofer ISI, 2017). In line with Reuß (2019), we make the following cost assumptions. Toll is set to 0.15 EUR/km. Drivers' wage is set to 35 EUR/h. Average driving speed is set to 50 km/h. Truck investment costs are set to 174,000 EUR (Fraunhofer ISI, 2017), with depreciation over eight years and 12% O&M costs. For tube trailers, investment costs and capacities per trailer are technology specific. They are set to 860,000 EUR and 4,300 kg_{H_2} for liquefied hydrogen (LH2), 660,000 EUR and 1,100 kg_{H_2} for gaseous hydrogen (GH2), and to 150,000 EUR and 1,620 kg_{H_2} for LOHC. Besides, we assume depreciation over twelve years and O&M costs of 2%, adopted from Reuß et al. (2019).

9.4.2 Electricity system data

We parametrize both the uniform zonal price and the nodal price electricity model with data for generation, consumption and the transmission grid in 2030. For this, we utilize the data set published by vom Scheidt et al. (2020). In the following, we briefly describe this data set. All data are more elaborately documented and available for free use under a Creative Commons license in vom Scheidt et al. (2020).

Transmission grid data

The transmission grid in 2030 is constructed from a reference model of the existing grid, which is enhanced with all the expansions and new installations until 2030 that have been announced by the German Federal Network Agency. The resulting final grid representation consists of 485 nodes and 663 lines. The transmission capacity of all 220 kV lines is set to 490 MW, and that of all 380 kV lines to 1700 MW, based on Egerer (2016) and Kießling et al. (2011).

Electricity demand data

For consumption, the hourly consumption forecast scenario EUCO30 is used (European Network of Transmission System Operators for Electricity, 2018). To improve consistency of grid and consumption data, these hourly values are re-scaled so that the annual total (577 TWh) matches the sum used in the official grid development plan (544 TWh) by the German regulator Bundesnetzagentur (2019a).

Next, these re-scaled hourly demand values are spatially disaggregated to NUTS-3 levels. For this disaggregation, the gross domestic product (GDP) and the population of a region serve as proxies for its future electricity consumption. The resulting NUTS-3 consumption time series are assigned to the nearest grid node.

Electricity generation data

For generation, estimation is differentiated between renewable, i.e. non-dispatchable generation and dispatchable generation.

For renewable generation, i.e. solar PV and wind, historical hourly generation data from the four national grid operators is used (Bundesnetzagentur, 2018). For the baseline scenario with no hydrogen, these hourly values are re-scaled so that the annual total generation from each generation technology matches the sum used in the grid development plan (Bundesnetzagentur, 2019a). This results in an annual generation of 86.7 TWh from solar PV (compared to a mean of 35.34 TWh over 2016-2018), and of 247.4 TWh from wind (compared to a mean of 108.6 TWh over 2016-2018). For the scenarios with hydrogen, we factor in the current discussion about "additionality" (Pototschnig, 2021), by further scaling up the capacity of solar PV and wind proportionally to the additional electricity demand for hydrogen production. Last, the re-scaled hourly generation values are spatially disaggregated. For this, we use the installed generation capacity per ZIP code as provided by the German TSOs (Deutsche Übertragungsnetzbetreiber, 2018). For a sensitivity scenario that considers a regional quota for new wind generation capacity, see Appendix G.

For dispatchable electricity generation capacity, all relevant plants for 2030 from the power plant list of the German grid regulator are used (Bundesnetzagentur, 2019b). For each plant, marginal costs are calculated, based on fuel type, estimated efficiency, and emission costs. A CO_2 price of 60 EUR/ton is assumed (Bundesregierung, 2019).

Both renewable generation time series and dispatchable power plants, along with their marginal costs are assigned to the nearest grid node. Note that this approach provides high spatial granularity, but comes at the costs of treating Germany as an isolated system without cross-border electricity lines. This can affect the results for electricity prices and redispatch in both directions, as noted by Xiong et al. (2021). Therefore, a geographic expansion – e.g. a European model – can be worthwhile future work, but requires substantial additional data procurement efforts if the high spatial granularity is to be upheld.[30]

9.5 Results and Discussion

Upon parametrizing the models presented in Chapter 9.3 with the case study data presented in Chapter 9.4, we run the models sequentially in three steps. First, we derive baseline results for the electricity system without hydrogen, including whole-

[30] A starting point could be the open network model PyPSA-Eur-Sec-30 that works with one node per country (Victoria et al., 2019).

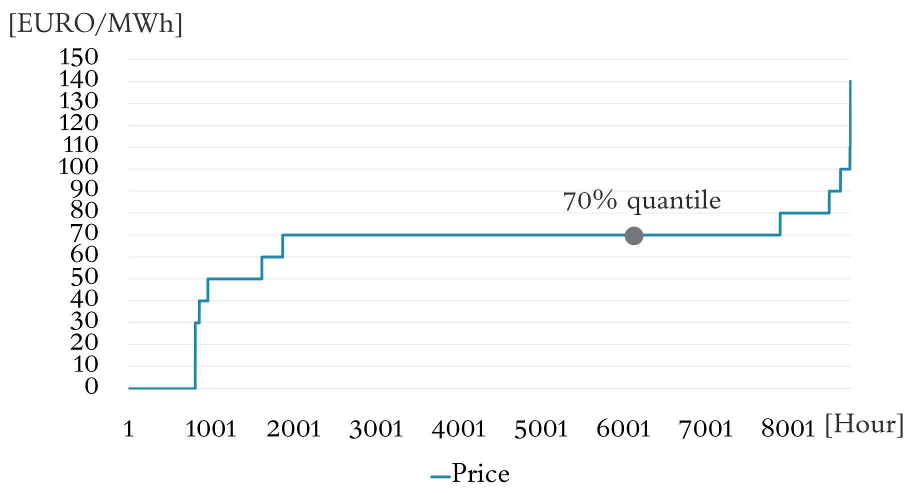


Figure 9.4.: Wholesale price duration curve in Germany, 2030 [EUR/MWh]

sale uniform zonal prices, nodal prices and congestion management costs (Chapter 9.5.1). Second, based on the resulting electricity tariffs, we derive information about the optimal hydrogen supply chains, including total end-use costs of hydrogen, as well as number, capacities and locations of electrolyzers (Chapter 9.5.2). Third, we observe the effects of integrating these hydrogen supply chains in the electricity system, including changes in total electricity demand, wholesale prices, redispatch costs, and CO_2 emissions (Chapter 9.5.3).

9.5.1 Baseline electricity system results

Without the integration of hydrogen, the resulting annual mean of the wholesale uniform price is 62.61 EUR/MWh. Figure 9.4 shows the price duration curve. The annual redispatch costs amount to 6.16 Billion EUR.

The resulting annual means of nodal prices vary between -54.30 and +221.00 EUR/MWh, with a median value of 67.80 EUR/MWh. Figure 9.5 shows the spatial distribution of nodal prices. Low prices are predominantly found in the North-East and North-West of the country, driven by high renewable generation and low demand. This finding is in line with Robinius et al. (2017), who analyze residual loads on county level and find negative residual loads predominantly in the North-East and North-West.[31]

[31] Neuhoff et al. (2013) calculate nodal prices for the year 2008 and find that prices vary between

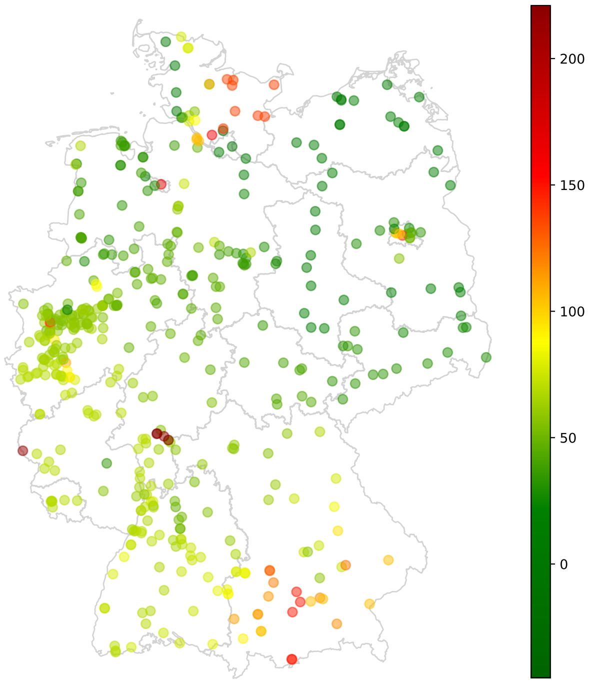


Figure 9.5.: Nodal prices in Germany, 2030 [EUR/MWh]

9.5.2 Hydrogen supply chain results

The resulting end-use costs for hydrogen are represented in Figure 9.6. As noted above, it is assumed that the tariff equals the wholesale electricity price, omitting grid fees, taxes, and other charges. In the uniform Flat scenario, which implies static electrolyzer operation under a time-invariant price, the final hydrogen costs for industry applications are 3.91 EUR/kg_{H_2} for LH2, 5.39 EUR/kg_{H_2} for GH2, and 4.21 EUR/kg_{H_2} for LOHC. For fuel cell trucks and cars, costs for fueling stations need to be added, resulting in final hydrogen costs of 4.01 EUR/kg_{H_2} for LH2, 5.53 EUR/kg_{H_2} for GH2, and 5.36 EUR/kg_{H_2} for LOHC. The largest share of costs is caused by production operation in all cases. These are largely driven by electricity costs (compare Eq. 9.4), which highlights the large role of electricity prices for the

10 and 100 EUR/MWh. The geographic disparity in the German generation system strongly increases from 2008 to 2030 due to a complete shut-down of all nuclear power plants, the partial shut-down of coal power plants, a strong renewable expansion especially in the North, and the introduction of a carbon emission price. This presumably causes the prices in our 2030 case study to have a larger (geographic) variance.

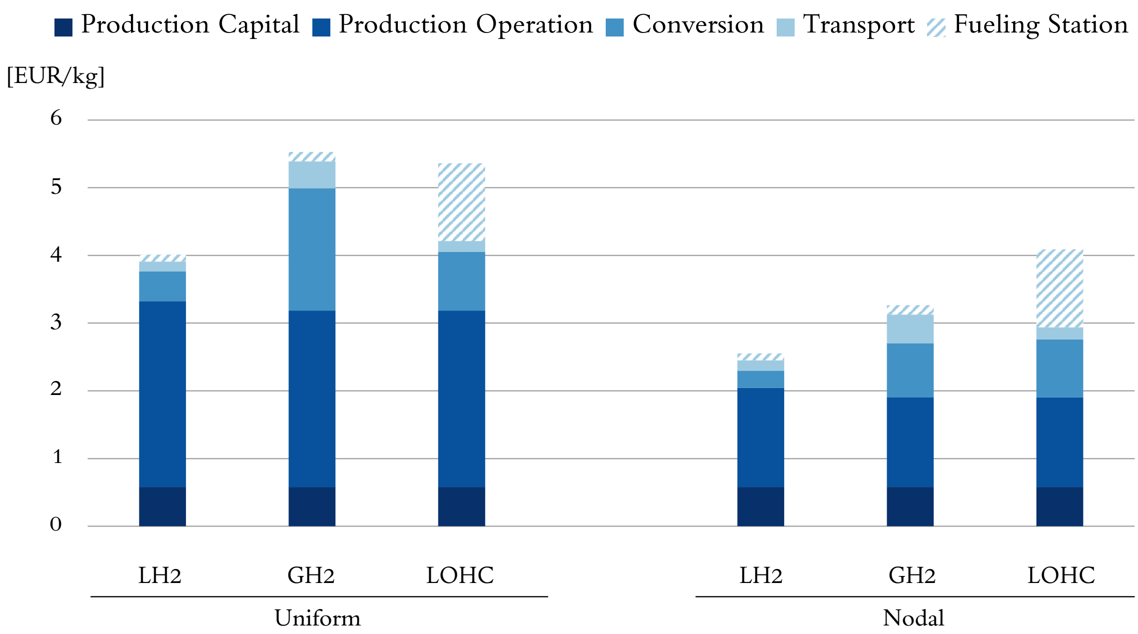


Figure 9.6.: End-use hydrogen costs by component and scenario: Effects of delivery form

end-use costs of electrolytic hydrogen.

This is also reflected by the results under the nodal tariff. In this case, the lower electricity costs for electrolyzers lead to much lower total hydrogen costs, i.e. to 2.45 (2.55 for fuel cell trucks and cars) EUR/kg_{H_2} for LH2, 3.13 (3.26) EUR/kg_{H_2} for GH2, and 2.94 (4.09) EUR/kg_{H_2} for LOHC.

For the cheapest delivery form, i.e. LH2, we additionally compute the scenarios with flexible operation. In these scenarios, electrolysis is shifted to hours with the lowest prices. For the uniform flexible case, electrolyzers are assumed to run at 100% capacity during the 70% cheapest hours at the wholesale market. For the nodal flexible case, electrolyzers are similarly assumed to run at 100% capacity during the 70% cheapest hours of the respective node.

This flexible operation enables electrolyzers to use cheaper electricity and thus leads to overall lower hydrogen costs, as Figure 9.7 shows. In the uniform case, flexible operation decreases total costs by 0.38 EUR/kg_{H_2}. In the nodal case, moving from static to flexible operation decreases costs by 0.58 EUR/kg_{H_2}.

The cost-minimal locations of electrolyzers are depicted in Figures 9.8 and 9.9.

The size of the markers corresponds to production volume. The largest marker in the North-West depicts overseas imports, which are exogenously determined (compare Chapter 9.4.1) and thus occur equally in all scenarios. In terms of domestic production, 9.50 GW_{el} of electrolysis capacity are installed in all scenarios with demand from industry, trucks, and cars.

Under uniform zonal tariffs with LH2, 101 domestic electrolyzers are placed. They are predominantly placed close to points of consumption, in order to minimize transportation costs (Figure 9.8). Half of the installed electrolyzers (52) have the maximal possible capacity of 100 MW. The siting is very similar for GH2 and LOHC, with 97, and 106 electrolyzers placed, respectively.

Under nodal tariffs, electrolyzers are placed further away from consumption, but at nodes with low electricity prices (Figure 9.9). This indicates that the cheaper electricity costs outweigh the higher transportation operating costs. This effect is stable across the three delivery states, and is in line with the findings from vom Scheidt et al. (2021), Robinius et al. (2017), and Jentsch et al. (2014). In the LH2 nodal case, 76 electrolyzers are placed, of which 63 have maximal possible capacity. Again, the siting is very similar for GH2 (69 electrolyzers), and LOHC (72).

In both scenarios, there are small differences between the three delivery states, which are caused by the different trailer capacities, different per-kg transport operating costs (see Eq. 9.12 to 9.15) and conversion operating costs (see Eq. 9.8 to 9.9). These in turn affect the optimal location of electrolyzers (compare Eq. 9.1).

9.5.3 Integration results

From the locations and capacities of electrolyzers presented above, we calculate the additional electricity demand from hydrogen production at each grid node. With this new input, we recalculate electricity prices and congestion management costs to identify the effects of hydrogen on the electricity system. For these calculations we assume LH2 delivery, since it is the cost-minimal hydrogen supply chain set-up in all scenarios, for both industry and transportation applications.

Table 9.9 summarizes the key results. The electrolytic production of hydrogen creates considerable new electricity demand of 72.49 TWh per year that increases the total national electricity demand by about 13%. Since this demand is assumed to

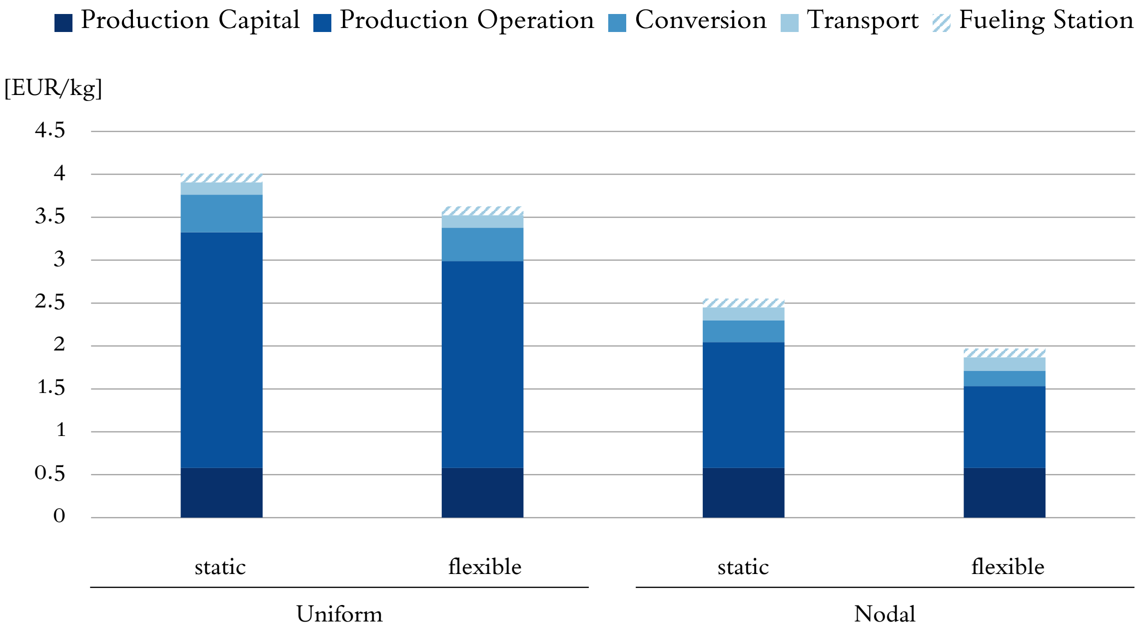
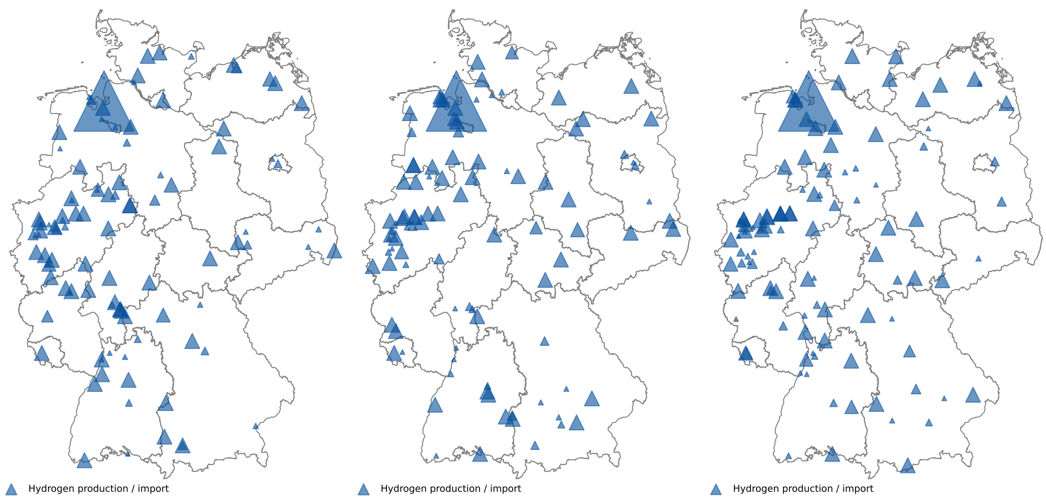
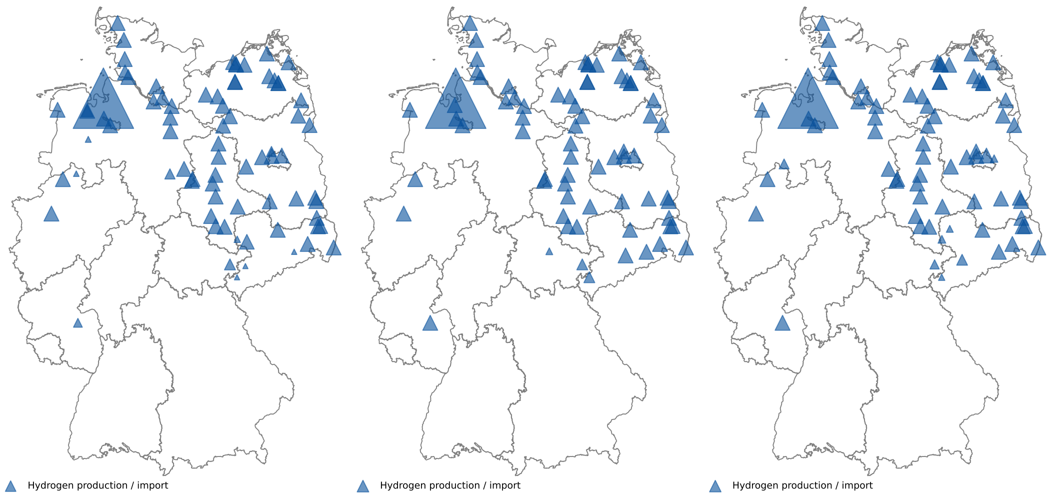


Figure 9.7.: End-use hydrogen costs by component and scenario: Effects of static versus flexible operation



(a) LH2 trailer delivery (b) GH2 trailer delivery (c) LOHC trailer delivery

Figure 9.8.: Optimal electrolyzer locations under uniform tariff



(a) LH2 trailer delivery (b) GH2 trailer delivery (c) LOHC trailer delivery

Figure 9.9.: Optimal electrolyzer locations under nodal tariff (static operation)

be met by additionally installed solar PV and wind capacity, the average electricity wholesale prices slightly decrease, by 4-7%, depending on the scenario.

If the hydrogen supply chain is optimized according to the uniform zonal tariff, annual congestion management costs *increase* by 17-18%. This corresponds to an increase of over one billion Euro per year. Interestingly, this increase is only slightly smaller for the uniform tariff with flexible operation, compared to the uniform tariff with static operation. This finding indicates that electrolyzers, which respond to real-time wholesale prices, but are inefficiently placed from a system perspective, might not be able to fully realize expected positive impacts regarding the actual use of cheap renewable energy (see e.g. (Ruhnau, 2020)) due to grid constraints. A key explanatory factor for this might be that wind generation, which to a large extend is located in the North of Germany (Deutsche Übertragungsnetzbetreiber, 2018), has been shown to drive wholesale prices down (Benhmad and Percebois, 2018) and at the same time drives congestion in the transmission grid (Staudt et al., 2019b). This finding is underlined by the fact that system-wide emissions increase under uniform tariffs, despite the expansion of renewable generation capacity to meet the demand from electrolyzers.

In contrast, when electrolyzers are placed and operated under nodal price signals, they *decrease* congestion management costs by 17-20% compared to the reference scenario. This decrease corresponds to over one billion Euro per year. In addition, nodal tariffs also lead to lower system emissions. The decrease in costs and emissions is larger under the nodal tariff with flexible operation, which shows that the combination of resolved spatial and temporal signals yields the largest benefits.

In summary, there is a delta of over two billion Euro and over five Megatons (Mt) of CO_2 per year between hydrogen integration under the status quo uniform price scenarios and under the nodal price scenarios. In other terms, the production of one kg_{H_2} on average creates additional congestion costs of 0.68-0.72 Euro under current regulation, whereas it reduces congestion costs by up to 0.82 Euro under more efficient regulation. This means, a spatially differentiated subsidy for hydrogen production – e.g. in the form of a per-kWh payment of the spread between uniform prices and simulated nodal prices – could effectively be covered by saved redispatch costs.

It is noteworthy, that the model does not assume that investors consider how their electrolyzer installation will affect nodal prices. This would require iterative calculation of both models, which is out of scope due to high computational effort. Regarding practical implementability, the complex and potentially vulnerable nature of nodal price signals represents another limitation. For hydrogen investors to base their decisions on nodal price signals, they need to be able to forecast these a priori, for which sufficient information and appropriate data analytics methods need to be available (vom Scheidt et al., 2020). Furthermore, investors face the risk of unforeseen expansion of grid or generation capacity that impacts nodal prices. Therefore, policy makers could opt to assess less efficient price signals such as more granular zonal tariffs and regionalized grid fees. Alternatively, non-price mechanisms are conceivable, such as regional quotas or allowing grid operators to curtail electrolyzers before performing the regular redispatch measures, in case of congestion. While such mechanisms typically forego some of the efficiency gains from nodal signals, they provide advantages regarding simplicity and associated risks. Therefore, it is desirable that future studies investigate the advantages and disadvantages of different (spatial) regulatory instruments.[32]

[32]For related analyzes regarding the integration of generation see e.g. Bertsch et al. (2015); Grimm et al. (2019); Schmidt and Zinke (2020). For a comprehensive review of locational investment signals for generation capacity that are applied in practice see Eicke et al. (2020).

Table 9.9.: Electricity demand, wholesale price and congestion management costs in 2030

Scenario	**Mean wholesale price [EUR/MWh]**	**Congestion management costs [MEUR/year]**	**CO_2 emissions [Mt/year]**
Baseline without H_2	62.61	6,163.96	59.1
With H_2, Uniform Tariff, Static operation	58.51 (-6.55%)	7,253.56 (+17.68%)	60.8 (+2.93%)
With H_2, Uniform Tariff, Flexible operation	59.91 (-4.31%)	7,203.11 (+16.86%)	61.3 (+3.73%)
With H_2, Nodal Tariff, Static operation	58.51 (-6.55%)	5,100.84 (-17.25%)	58.4 (-1.26%)
With H_2, Nodal Tariff, Flexible operation	59.24 (-5.38%)	4,915.41 (-20.26%)	55.6 (-5.85%)

Last, the generalizability of our findings to certain other geographies is limited by the focus on one technology for hydrogen production, i.e. electrolysis. Hydrogen from steam methane reforming with carbon capture and storage and rigorous methane leakage prevention represents a (transitional) alternative of producing hydrogen with net neutral emissions and can be an economic alternative to electrolytic hydrogen, depending on political and geographic circumstances (see e.g. Bødal et al. (2020)). In the German case, however, political action is strongly focused on electrolysis (Bundesregierung, 2020).

9.6 Conclusions and Policy Implications

Policymakers in dozens of countries are currently planning public funding for the development of future hydrogen infrastructure, with growing interest in electricity based hydrogen production. The large-scale deployment of electrolytic hydrogen is likely to have a large effect on the planning and operation of electricity systems. Our study sheds light on the spatial interaction between hydrogen infrastructure reliant on electrolytic hydrogen and the power system.

For this, we propose a three-step methodology based on linking an electricity system dispatch model and a hydrogen supply chain model, both with granular spatial resolution. We apply this methodology to a case study of the German system in 2030.

In the first step, we use an electricity system dispatch model to simulate uniform zonal electricity prices – representing current German regulation – and nodal prices, without considering hydrogen demand and production.

In the second step, we feed those prices into the hydrogen model, together with additional techno-economic parameters for capital and operation costs. This way, we determine the optimal spatial design of hydrogen supply chains under current uniform regulation and a regulation with efficient spatial price signals. We identify liquefied hydrogen as the most economical form of truck based hydrogen delivery in all scenarios. Furthermore, we find that under the existing uniform zonal electricity pricing paradigm, electrolyzers are cost-minimally placed close to consumption points, such as industry plants and large cities. In the nodal pricing scenario, we find that the price differences among nodes are large enough to move hydrogen production to low-cost nodes that are further away from consumption points and closer to low-cost electricity generation capacity.

In the third step, we feed back the resulting electric loads from electrolyzers into the electricity system dispatch model. The results show that the integration of hydrogen under current uniform prices causes a large increase in congestion management costs of about 17%, or one billion Euro per year. Moreover, emissions are increased by 3-4%, or about two Megatons per year. Thus, our analysis shows that the existing inefficiencies of single-price zonal markets can be strongly aggravated by hydrogen. Given efficient spatial economic signals, electrolyzers are integrated in a much more system-friendly way, causing a decrease in congestion management costs of up to 20%, or about 1.1 billion Euro per year, compared to the benchmark scenario without hydrogen. Moreover, CO_2 emissions are decreased by up to 6%. When comparing the impacts of spatial (uniform vs. nodal) vs. temporal (static vs. flexible) signals on congestion management costs, our results indicate that introducing spatial variance in price signals has substantially higher benefits. The largest cost reduction can be achieved when both dimensions are combined, i.e. in a nodal real-time price signal that incentivizes flexible operation.

This is important information for policy makers in single-price zonal electricity markets, such as Germany, that intend to subsidize electrolytic hydrogen production, as our results demonstrate the considerable benefits of spatially differentiated subsidies. In fact, the subsidies a regulator would have to pay to mimic nodal prices for hydrogen within the existing single-price market design could effectively be covered from avoided redispatch costs.

Given prevailing political barriers to introducing nodal pricing markets in Europe (European Network of Transmission System Operators for Electricity, 2021), it is important to note that policy makers can incorporate our findings within the existing single-price zonal markets. For instance, they could design a specific nodal tariff, which bills electrolyzers based on shadow nodal prices instead of wholesale prices. Alternatively, per-kWh subsidies (see (Bundesregierung, 2020)), can be differentiated by grid node, mimicking the spread between uniform prices and simulated nodal prices. Other locational incentives like regional quotas, regionalized grid fees, or allowing grid operators to curtail electrolyzers before performing the regular redispatch measures should be analyzed in future work regarding their economic efficiency and other politically relevant criteria. As our study quantifies the large potential benefits of a holistic integration of hydrogen in single-price zonal electricity systems, it also motivates future investigations into the solution space of regulatory mechanisms.

In summary, this Part III complements the prior Part II in two important aspects. First, it demonstrates that tariffs do not only affect technology integration at the customer level, but also cause important effects on the system. Second, it showcases the considerable benefits of tariffs with temporal *and* spatial granularity.

Part IV.

Finale

CHAPTER 10

CONTRIBUTIONS AND IMPLICATIONS

Depending on their design, electricity tariffs can have large effects, both positive or negative, on the societal costs of energy systems. These effects will be amplified by the transition to an electrified energy system. To facilitate a successful integration of new electric technologies, I conduct various analyses that extend our knowledge about the interplay of tariffs and technology integration. For this, I engineer tariffs and tariff recommendation methods and evaluate them in quantitative case studies. In this chapter, I summarize the answers to the nine research questions posed in Chapter 2 and distill the core contributions and implications for stakeholders in electricity markets.

The high potential benefits of economically efficient residential electricity tariffs, together with their low adoption rates in many geographies motivate the development and assessment of tariff recommendation methods. Research questions 1-4 address this challenge.

With respect to Research Question 1 (*"What is the performance of a naive tariff recommendation approach based on historical data?"*), the performance of the recommendation approach is evaluated by precision, recall, and F1-score on a data set of residential customers from Chicago, USA. All measures differ depending on the analyzed tariff. Precision or recall are never higher than 0.60. The F1-score, which combines precision and recall, is between 0.08 and 0.43 and thus, far from the potential maximum value of 1. By introducing a tariff confusion matrix, it is found that the hourly TOU ("TOU-24") and the RTP tariff are most likely to be confused. In summary, the performance of the naive approach is unsatisfying, as it can cause increased (opportunity) costs for consumers and therefore reduce trust in the recommendation. The answer to Research Question 1 therefore motivates further research that applies more sophisticated methods to increase tariff recommendation quality, as addressed in Research Question 3 and 4.

Regarding Research Question 2 (*"What are the economic consequences of these recommendations for customers?"*), findings show that the economic consequences of tariff selection based on the naive approach are small for most customers. The median extra costs for selecting sub-optimal tariffs vary from 0.2 to 10.6 Euro per year. The highest extra costs occur for consumers who wrongfully select the RTP tariff. However, the small size of economic consequences is not necessarily due to the quality of recommendation, but rather the general limited spread in electricity bills under different tariffs. For instance, over 90% of customers have a total savings potential of under 22 Euro per year. This motivates future research that expands tariff-only recommendations to tariff-and-technology bundle recommendations to increase potential customer savings. Besides, one central methodical limitation is that price response is ignored, which limits the savings potential. Therefore, price response is incorporated in the method of the subsequent chapter that addresses Research Question 3 and 4.[33]

Building on the insights from the answers to Research Question 1, I address Research Question 3 (*"What is the performance of Machine Learning based methods for recommending bundles of tariffs and technologies to end-consumers?"*). For a case study of residential customers from London, UK, I find that the developed Machine Learning methods achieve accuracies of 73-76% for recommendations of bundles that consist of tariffs and residential electric technologies. Thus, these methods largely outperform the naive benchmark that achieves an accuracy of 56%. Moreover, the results demonstrate that using four week long excerpts of customers' smart meter data as input has a crucial impact on the performance of Machine Learning methods. For instance, the XGBoost model's accuracy is only slightly better than the naive benchmark without the smart meter data (59%). Due to the prevailing lack of multi year data sets, this analysis is based on one case study. This represents a limitation and once more data sets become available, the developed recommendation model can be applied to them to verify the model's performance across a broader range of

[33]Results converted from US Dollar to Euro for better comparability. The conversion assumes an exchange ratio of 1 USD = 0.879468 EUR.

regions and time periods.

With respect to Research Question 4 (*"What are the economic consequences of these recommendations for customers?"*), the results show that while the average customer pays 3,535 Euro for their electricity, mobility, and heating per year in the status quo, the best Machine Learning recommendation method can reduce this to 3,151 Euro per year. The delta, i.e. 384 Euro, is substantially larger than the delta achieved by the naive tariff-only recommender. Similar to the statistical evaluation, the economic evaluation shows that using four week long excerpts of customers' smart meter data is beneficial. Without such data, average savings from the recommended bundles are 24 Euro lower. The holistic assessment of statistical and economic performance uncovers that the chosen metric for the Machine Learning models, i.e. accuracy, is not a perfect proxy for costs, since small accuracy improvements over the naive method already capture the majority of the economic savings. Therefore, future studies could develop a customized loss function for the bundle recommendation task to further improve the models' performance regarding economic consequences for customers.[34]

The analysis conducted to answer Research Question 4 also shows the high potential of operating residential electric technologies according to time-varying electricity tariffs. One limitation of the technology scheduling model is the assumption that a customer's base load of the next 24 hours is known. To schedule technologies in practice, adequate forecasting methods for residential loads are required. In that respect, I address Research Question 5 (*"What are state of the art methodological approaches for electric load forecasting in the literature?"*) by reviewing the status quo of short-term residential and building electricity consumption forecasting. The review shows that the state of the art methodological approaches are Machine Learning models and probabilistic approaches. Besides, to ensure research rigour and replicability, forecasters should select input features carefully, compare various approaches in their work, use (or create) public reference data sets, and apply prevalent error measures.

Based on these findings, I develop a novel, pinball loss guided probabilistic Machine Learning forecasting model based on Gated Recurrent Units. Since

[34]Results converted from British Pound to Euro for better comparability. The conversion assumes an exchange ratio of 1 GBP = 1.18937 EUR.

forecasting electricity consumption of households with distributed energy technologies represents an important gap in the existing body of literature, I apply this model to a case study of US households with solar PV installations, electric heating, and both. This enables me to answer Research Question 6 (*"What is the performance of Machine Learning sequence models for forecasting residential electric loads in the presence of roof-top solar and electric heating installations?"*). The results show that the forecasts have the best performance for households with solar PV (mean pinball loss of 0.14 kWh), and worst performance for households with electric heating (mean pinball loss of 0.22 kWh). The latter result could be caused to the limited length of the training data set that only encompasses one heating season. The novel proposed forecasting model performs better than the benchmark models for customers with solar PV, electric heating, and both technologies. These are the first academic findings for probabilistic forecasting of household loads under the influence of distributed energy technologies and thus lay important foundations. Future work can build on these foundations by replicating the analysis on longer time series and by demonstrating the application of such forecasts in energy management systems like to one developed in Chapter 6 of this thesis.

In summary, the research in Part II of this thesis contributes multiple novel insights into the role of electricity tariffs for integrated energy systems at the customer level. Its key contributions are the development of novel, data-driven methods for tariff recommendation and net load forecasting and the demonstration of how they can foster the proliferation of more economically efficient electricity tariffs and sustainable energy technologies amongst residential customers. This has several concrete practical implications. The developed decision support tool helps residential customers to find their personalized, cost-optimal energy service bundle and thus enables individual cost savings. As time-varying tariffs set more economically efficient signals for the operation of energy technologies than conventional Flat tariffs, their adoption also yields benefits for the system, e.g. by reducing peak loads and costs. To enable the scheduling of technologies in practice, this thesis in addition develops the first probabilistic forecasting model for net electricity loads of customers with novel residential electric technologies. Besides, the bundle recommendation generally supports the diffusion of sustainable technologies and smart meters, which are important for the energy transition. Moreover, the thesis shows how Machine Learning tools may help retailers in their business model transition in a strongly competitive retail market, by unlocking new cross-selling opportunities and facilitating the often criticized slow smart meter roll-out (see Chapter 3). Last, since this thesis reveals that if customers disclose certain individual data to their retailer, they can improve the accuracy of their recommendations, it brings forward the innovative concept of collaboration between customers and retailers for added value on both sides.

Research questions 1-6 concern the interplay of tariffs and small-scale technologies at the local level. They are therefore complemented by Research Questions 7-9, which concern the interplay of tariffs and large consumers at the system level and in the particular analyzed case, hydrogen electrolysis capacity.

In order to assess the impact of tariffs on the hydrogen supply chain in Germany, I first develop a comprehensive new hydrogen integration model and answer Research Question 7 (*"What is the cost-minimal supply chain design using electrolytic hydrogen production for the combined hydrogen demand from all major relevant sectors in 2030 in Germany?"*). The supply chain model includes hydrogen production, conversion, truck based transportation, reconversion, and in the case of trucks and cars, fueling. Hydrogen storage and pipeline transport are neglected, but can be added to the model if it is to be applied to scenarios with higher hydrogen volumes beyond 2030. The results show that 9.50 GW_{el} of electrolysis capacity are required to meet the estimated hydrogen demand from industry, trucks, and cars in 2030. This capacity is distributed over 69-106 electrolyzers, depending on the scenario. Transporting hydrogen in its liquefied state in delivery trucks is more economical than truck based transport of hydrogen in its gaseous state or hydrogen that is bound in LOHC.

To analyze the effect of tariffs on hydrogen supply chains, Research Question 8 (*"What is the effect of electricity tariffs on cost-minimal locations of electrolyzers and hydrogen costs?"*) is addressed. The analysis uncovers strong effects under the assumption that investors are risk neutral and have perfect foresight. Under uniform zonal tariffs, more, smaller electrolyzers are installed, and they are placed close to points of consumption. In contrast, under nodal tariffs, electrolyzers are instead placed at nodes with low electricity prices in all delivery scenarios. This demonstrates that the cheaper electricity costs at remote nodes realized by nodal tariffs robustly outweigh the higher transportation operating costs.

Last, to analyze the impact of tariffs on the feedback effects of hydrogen supply chains on the electricity system, Research Question 9 is answered (*"How does hydrogen production change electricity wholesale prices, congestion management costs, and CO_2 emissions under different tariffs?"*). In this regard, the results show that electrolytic production of hydrogen introduces a considerable additional electricity demand of 72 TWh annually to the wholesale market. If this new demand is fully covered by additionally installed solar PV and wind power capacity, average wholesale prices are not affected strongly, and even slightly decrease. Large tariff effects can be observed regarding congestion management costs and emissions. With the uniform zonal tariff, hydrogen increases annual congestion management costs by over one billion Euro and CO_2 emissions by 1.7-2.2 Megatons. However, if integrated according to the nodal tariff, hydrogen decreases congestion management costs by over one billion Euro per year, and emissions decrease by 0.7-3.5 Megatons. The findings indicate that for system integration, the location of electrolyzers is crucial. The least-cost and least-emission integration is achieved when the tariff contains both spatial and temporal signals.

In summary, the research in Part III of this thesis contributes multiple novel insights into the role of electricity tariffs for integrated energy systems at the system level. Its main contribution is the demonstration of the great value of spatially resolved electricity tariffs for hydrogen integration. The thesis thus showcases that efficient electricity tariffs are a powerful tool to align individual and societal interests in integrated energy systems. This has important implications for policy makers and regulators in dozens of single-price zonal electricity markets worldwide, who are currently planning subsidy schemes for electrolytic hydrogen production. The results clearly demonstrate the substantial benefits that policy makers and regulators can achieve by differentiating such subsidies according to spatial criteria. In the presented analysis of the German system, the required subsidies a regulator would have to pay to mimic nodal prices for hydrogen could effectively be covered from avoided redispatch costs.

This dissertation purposefully enhances our knowledge about electricity tariffs with a dedicated focus on the interplay of tariffs and novel electric technologies, such as hydrogen, heat pumps, and electric vehicles. It demonstrates that electricity tariffs with high temporal and spatial granularity for residential and industrial consumers are key coordination mechanisms for the beginning era of consumer-centric, integrated energy systems. It provides guidance for policy makers, market operators, regulators, and retailers who aim to engineer the next generation of electricity tariffs and related recommendation and forecasting tools.

CHAPTER 11

OUTLOOK

Based on the work provided in this thesis, promising pathways for future research are uncovered.

With respect to residential tariff recommendation, three main avenues for future work present themselves. First, customer acceptance of recommendations is an important issue. In reality, transaction costs and behavioral considerations influence customers' decisions of selecting tariffs or service bundles. For instance, behavioral economics in other contexts has found that people tend to frame decisions in terms of the default setting (i.e. a Flat tariff) and aim to avoid potential losses compared to that benchmark default setting (Dinner et al., 2011). Therefore, it can be interesting to evaluate the influence not only of the quality of the recommendation, but also of its display and framing (i.e. non-monetary "nudges") on tariff adoption among consumers. Besides such non-financial mechanisms, this loss aversion of many consumers also inspires the development of hedging mechanisms for service bundle recommendations. For this, future research could investigate how a "bill protection", i.e. a guarantee for non-increased costs could improve customer acceptance and how it could be best designed from the point of view of a retailer. Methodologically, these questions could be addressed by conducting controlled laboratory experiments.

Second, the detailed design of a new energy retailer business model is a highly relevant task, as uncovered in Chapter 3. For this, it is beneficial to extend this work by investigating the "behind-the-scenes" processes at the retailer that are needed to realize the presented new business model. For example, for customers who use real-time tariffs, electricity retailers could use automated agents based on Deep Reinforcement

Learning that manage the electricity procurement at the wholesale market in real-time, based on measured live customer data. Other aspects to be investigated are the lease of technologies in collaboration with hardware suppliers, and the collaboration for data sharing with customers.

Third, field experiments with a *Citizen Science* approach can drive the developed concept towards a real product for retail companies. For this, researchers could cooperate with citizens and retailers. Together, they can set up small sensor devices at the citizens' homes and record electricity consumption from conventional meters via optical interfaces. By using latest Transfer Learning approaches from the field of Artificial Intelligence, the recommendation models trained in this thesis can be applied even to small sets of measured empirical data, and real recommendations can be made. Moreover, forecasts based on Machine Learning methods are to be developed as inputs for the daily optimization of smart home energy systems. This way, the technical implementation in real-world settings can be tested. Thus, the idea conceived in this thesis can be realized in practice.

With respect to hydrogen regulation, I see three main directions in which this work can be pursued further.

First, regarding mechanism design, nodal prices represent the theoretical optimal mechanism for pricing electricity in an economically efficient manner. However, policy makers and regulators often aim to strike a balance between economic efficiency and other relevant objectives such as distributional effects (Burger et al., 2020), simplicity, investment risk, market power, and liquidity (Eicke and Schittekatte, 2022). Therefore, it is valuable to broaden the assessment of hydrogen integration effects to include such criteria and to assess how nodal tariffs and alternative mechanisms perform across them. Common types of mechanisms in electricity systems are price based mechanisms, volume based mechanisms, and direct control mechanisms. In the case of electrolyzers, price based alternatives to nodal tariffs are more granular zonal tariffs or regionalized grid fees that signal potential for congestion. Volume based mechanisms could be implemented as a “Northeast Quota” in Germany, which demands a minimum share of electrolysis capacity to be installed in northeastern states. This corresponds to the existing "Southern Quota" for new wind turbine installations (see Appendix G). Direct control mechanisms for electrolyzers could be realized by allowing grid operators to curtail electrolyzers before performing the regular redispatch measures, in case of congestion. Simulating and comparing a range of mechanisms across multiple objectives will provide valuable guidance for policy makers.

Second, methodically, the hydrogen supply chain model presented in this thesis could be reformulated as an agent based model and linked to existing agent based electricity system models (Weidlich and Veit, 2008). With such an approach, one could capture the effects of various risk attitudes and incomplete information among hydrogen infrastructure investors and system planners.

Third, the increasing regional integration of European electricity systems motivates future work that expands the regional scope of the presented analysis. For example, beyond 2030, there will likely be hydrogen trade between European countries. For such trade, alternative transportation means like ships and pipelines should be assessed. In addition, at nodes that are not connected to the rest of the electric grid, e.g. off-shore wind parks in the North Sea, hydrogen could be produced on-site and filled into tankers or pipelines for transport. Such complex and geographically extensive hydrogen supply chains will demand newly engineered economic mechanisms. In addition, state of the art methods from the field of Artificial Intelligence can deliver solutions for the newly evolving optimization and forecasting tasks. Together, well-engineered mechanisms, optimization models, and forecasts can ensure an economically efficient, sustainable, and secure energy system integration.

As this thesis demonstrates the importance of electricity tariffs for the beginning era of integrated energy systems, it also motivates further research for unlocking their full potential.

Appendices

APPENDIX A

ELECTROLYSIS CAPACITY IN GERMANY

Table A.1.: Installed and planned electrolysis capacity in Germany

Project name	City/Region	Technology	Commissioning year	Rated capacity [kW]
HYSOLAR	Stuttgart	AEC	1989	45.0
PHOEBUS Jülich	Jülich	AEC	1994	26.0
CUTE	Hamburg	AEC	2003	390.0
ARGE Wasserstoff-Initiative-Vorpommern	Barth	PEM	2005	62.0
VW Hydrogen filling station	Isenbüttel	PEM	2005	6.1
Hydrogen filling station Holzmarktstraße	Berlin	AEC	2010	310.0
Juwi laboratory plant	Morbach	Unknown	2011	25.0
Hybrid Power Plant Prenzlau	Prenzlau	AEC	2011	560.0
Prototype BTU	Cottbus	AEC	2012	140.0
H2 Move - Hydrogen filling station	Freiburg	PEM	2012	42.0
RH2-WKA Project	Grapzow	AEC	2012	1,000.0
Power-to-Gas Plant Viessmann	Schwandorf	PEM	2012	108.0
Hydrogen filling station Talstraße (only cars)	Stuttgart	AEC	2012	320.0

Table A.1.: Installed and planned electrolysis capacity in Germany (continued)

Project name	City/Region	Techno-logy	Commis-sioning year	Rated capacity [kW]
WindGas Falkenhagen	Falkenhagen	AEC	2013	2,000.0
Hydrogen filling station HafenCity	Hamburg	AEC	2013	600.0
CO2RRECT	Niederaußem	PEM	2013	300.0
Audi e-gas	Werlte	AEC	2013	6,300.0
Strom zu Gas-Anlage (Thüga-Gruppe)	Frankfurt am Main	PEM	2014	325.0
Hydrogen filling station Talstraße (cars & trucks)	Stuttgart	AEC	2014	320.0
BioPower2Gas	Allendorf (Eder)	PEM	2015	300.0
Smart Grid Solar	Arzberg	PEM	2015	75.0
Hydrogen filling station H2BER	Berlin	AEC	2015	650.0
Hydrogen filling station Schnackenburgallee	Hamburg	PEM	2015	180.0
PtG Ibbenbüren	Ibbenbüren	PEM	2015	200.0
SOPHIA	Köln	SOEC	2015	4.8
Energiepark Mainz	Mainz	PEM	2015	6,000.0
WindGas Hamburg	Reitbrook	PEM	2015	1,500.0
Stromlückenfüller	Reußenköge	PEM	2015	37.5
Exytron	Rostock	AEC	2015	21.0
Windgas Haßfurt	Haßfurt	PEM	2016	1,250.0
Direktmethanisierung von Biogas	Bad Hersfeld	PEM	2017	50.0
Hydrogen Feed-in Plant	Freiburg	PEM	2017	120.0
Hydrogen filling station Erlachseeweg	Karlsruhe	SOEC	2017	7.9
Stromlückenfüller Expansion	Reußenköge	PEM	2017	330.0

Table A.1.: Installed and planned electrolysis capacity in Germany (continued)

Project name	City/Region	Techno-logy	Commis-sioning year	Rated capacity [kW]
Projekt GrInHy 1.0 (Green Industry Hydrogen)	Salzgitter	SOEC	2017	200.0
Wind2Gas Energy Wasserstoff Elektrolyse	Brunsbüttel	PEM	2018	2,400.0
Carbon2Chem-Technikum	Duisburg	AEC	2018	2,000.0
Zero Emission Wohnpark Alzey	Alzey	AEC	2019	62.5
Klimafreundliches Wohnen in Augsburg	Augsburg	AEC	2019	62.5
HPEM2GAS Project	Emden	PEM	2019	200.0
Leuchtturmprojekt Power-to-Gas	Grenzach-Wyhlen	AEC	2019	1,000.0
LocalHy	Sonneberg-Heubisch	AEC	2019	75.0
Self-sufficient operating site Westnetz	Metelen	PEM	2019	14.6
Windgas Haurup	Haurup	PEM	2020	1,000.0
Projekt GrInHy 2.0 (Green Industry Hydrogen)	Salzgitter	SOEC	2020	720.0
Windwasserstoff Salzgitter	Salzgitter	PEM	2020	2,200.0
Bernsteinsee Hotel	Sassenburg/Stüde	AEC	2020	52.0
H2ORIZON	Lampoldshausen	PEM	2020	880.0
rSOC Project	Dresden	SOEC	2021	180.0
Clean Energy Conversion	Haren	PEM	2021	4,000.0
Öhringer Wasserstoffinsel	Öhringen	AEC	2021	300.0
Energiepark Pirmasens-Winzeln	Pirmasens	Unknown	2021	1,800.0

Table A.1.: Installed and planned electrolysis capacity in Germany (continued)

Project name	City/Region	Technology	Commissioning year	Rated capacity [kW]
eFarm Project	Reußenköge, Bosbüll, Langenhorn, Dörpum	PEM	2021	1,650.0
REFHYNE	Wesseling	PEM	2021	10,000.0
H2-Project Ellhöft	Westre/Ellhöft	PEM	2021	330.0
Wunsiedler Energiepark	Wunsiedel	PEM	2021	6,000.0
ELEMENT EINS	Diele (recommended)	AEC	2022	100,000.0
Westküste100	Heide	Unknown	2022	30,000.0
Energiepark Bad Lauchstädt	Bad Lauchstädt	Unknown	2023	35,000.0
GET H2 Nukleus	Lingen	Unknown	2023	100,000.0
HydroHub Fenne	Fenne	PEM	2024	17,500.0
GreenHydroChem Mitteldeutschland	Leuna	Unknown	2024	100,000.0

APPENDIX B

EXPERT INTERVIEW QUESTIONS

- "If you could wish for one change of regulation, what would it be?" (Original: "Wenn Sie sich eine Regulierungsänderung wünschen könnten, welche wäre das?)
- "Which possibilities do you see in the area of cross-selling of tariffs and technologies?" (Original: "Welche Möglichkeiten sehen Sie im Bereich Cross-Selling von Tarifen und Technologien?)
- "Which possibilities do you see regarding servitization in the electricity retail market and which services, as an add-on for the product electricity, are especially relevant and in demand?" (Original: "Welche Möglichkeiten sehen Sie bezüglich Servitization im Endkundenmarkt für Strom und welche Dienstleistungen, als Zusatz zum Produkt Strom sind für Stromkunden im Endkundenmarkt besonders relevant und gefragt?")
- "Which role do transaction costs play for the probability and frequency of switching tariffs? How could such transaction costs be reduced?" (Original: "Welche Rolle spielen Transaktionskosten für die Wechselwahrscheinlichkeit und -häufigkeit bei Tarifen? Wie können solche Transaktionskosten reduziert werden?)
- "Which role do online sales channels play compared to offline sales channels in the retail market?" (Original: "Welche Rolle spielen Online-Vertriebskanäle im Vergleich zu Offline-Vertriebskanälen im Endkundenmarkt?)
- "Besides fixed and flat price components, which characteristics of tariffs are

important to retailers?" (Original: "Neben Grund- und Arbeitspreisen, welche Eigenschaften eines Tarifes sind Anbietern wichtig?)

- "Besides fixed and flat price components, which characteristics of tariffs are important to customers?" (Original: "Neben Grund- und Arbeitspreisen, welche Eigenschaften eines Tarifes sind Kunden wichtig?)
- "Into which types/groups of private customers can the retail market be divided?" (Original: "In welche unterschiedlichen Typen/Gruppen von privaten Kunden kann der Endkundenmarkt aufgeteilt werden?)
- "Which importance do partnerships with other companies have?" (Original: "Welche Bedeutung haben Partnerschaften mit anderen Unternehmen?)
- "How does the interplay of processes for electricity purchasing and selling work for the retailers? What role do Futures, Forwards, OTC, day ahead and intra day trading play? Which particular complexity regarding these processes evolves in the case of innovative tariffs (e.g. time-varying, eco)? How can one automate the short-term procurement (e.g. in the day-ahead market)?" (Original: "Wie funktioniert bei Anbietern das Zusammenspiel von Prozessen für Stromeinkauf und -vertrieb? Welche Rollen spielen bei der Beschaffung jeweils Futures, Forwards, OTC-, Dayahead- und Intraday-Handel? Welche besondere Komplexität hinsichtlich dieser Prozesse entsteht bei neuartigen Tarifen (z.B. zeitvariabel, Ökostrom)? Wie kann man die kurzfristigere Beschaffung (z.B. am Day-Ahead Markt) für zeitvariable Tarife automatisieren?)

APPENDIX C

TARIFF RECOMMENDATION CASE STUDY DATA

C.1 Consumption Data

Among the electricity consumption profiles, a minimum annual consumption of 1,026.50 kWh and a maximum value of 9,753.05 kWh can be observed, in the first year. In the second year, the annual consumption is between 1,001.91 kWh and 11,500.73 kWh. Figure A.1 display the distribution of the annual consumption values.

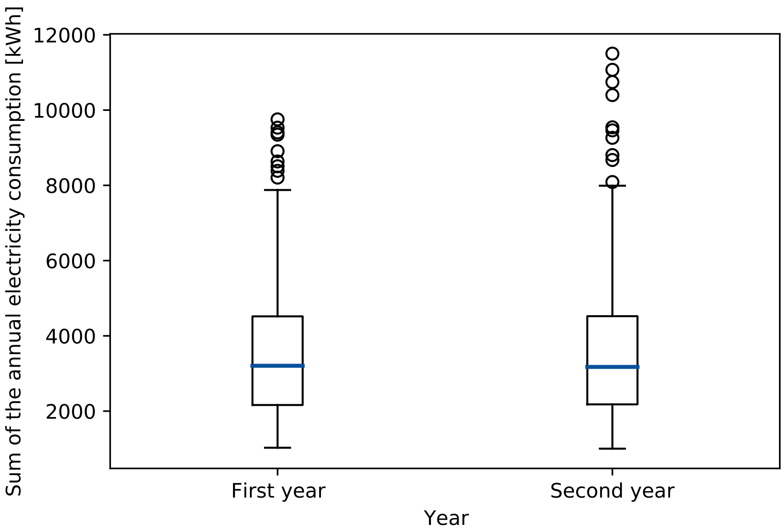


Figure A.1.: Distribution of the annual electricity consumption of the households

C.2 Electricity Tariffs

In the data of 2018, two data points are missing. In 2019, 26 data points are missing. They are supplemented by linear interpolation. Figure A.2 shows the distribution of wholesale electricity prices in 2018 across the hours of a day in the form of box plots. Figure A.3 illustrates the distribution of the same data in 2019. For the application, the price data of 2018 is linked to the consumption data of 2012 to form the first year's data and the 2019 price data is linked to the 2013 consumption data to form the second year's data.

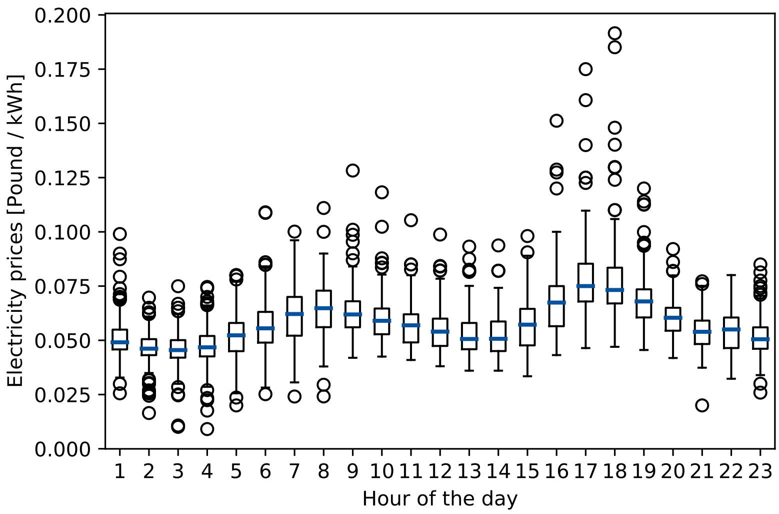


Figure A.2.: First year's hourly electricity wholesale prices in the UK throughout the day

Equation C.1 defines the calculation of the electricity price for the flat tariff ep^{flat}.

$$ep_t^{flat} = \frac{\sum_{d=1}^{365} \sum_{h=1}^{24} wp_{d,h} \cdot y_{d,h}}{\sum_{d=1}^{365} \sum_{h=1}^{24} y_{d,h}}, \quad t \in [1, 8760] \tag{C.1}$$

For the TOU-2 tariff, the energy prices are determined according to C.2 and C.3. Equation C.4 sets the time periods in which these prices occur.

$$ep^{tou2,l1} = \frac{\sum_{d=1}^{365} (\sum_{h=1}^{6} wp_{d,h} \cdot y_{d,h} + \sum_{h=23}^{24} wp_{d,h} \cdot y_{d,h})}{\sum_{d=1}^{365} (\sum_{h=1}^{6} y_{d,h} + \sum_{h=23}^{24} y_{d,h})} \tag{C.2}$$

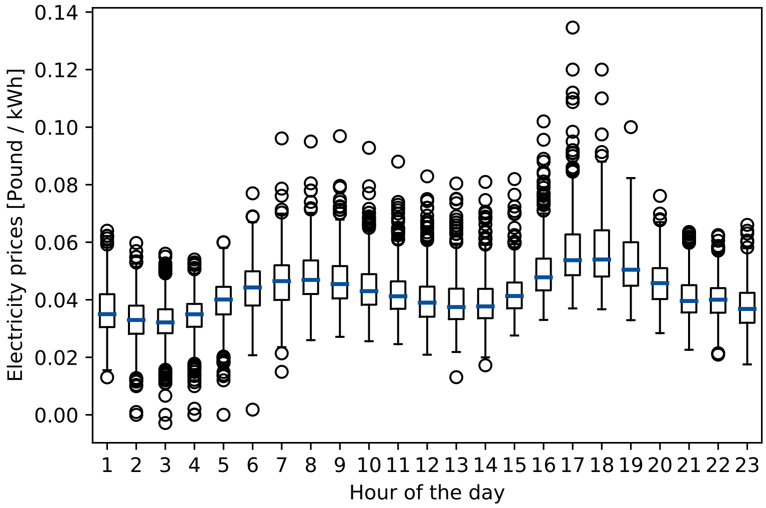


Figure A.3.: Second year's hourly electricity wholesale prices in the UK throughout the day

$$ep^{tou2,l2} = \frac{\sum_{d=1}^{365} \sum_{h=7}^{22} wp_{d,h} \cdot y_{d,h}}{\sum_{d=1}^{365} \sum_{h=7}^{22} y_{d,h}} \tag{C.3}$$

$$ep_t^{tou2} = \begin{cases} ep^{tou2,l1}, & \text{if } t \in [24k+1,\ 24k+6] \\ & \bigsqcup [24k+23,\ 24k+24] \\ & \text{with } k \in [0, 364] \\ ep^{tou2,l2}, & \text{if } t \in [24k+7,\ 24k+22] \\ & \text{with } k \in [0, 364] \end{cases} \tag{C.4}$$

The calculation of the three TOU-3 price levels is conducted similarly to the TOU-2, as shown in Equations C.5, C.6, and C.7. Equation C.8 sets the time periods in which these prices occur.

$$ep^{tou3,l1} = \frac{\sum_{d=1}^{365} (\sum_{h=1}^{6} wp_{d,h} \cdot y_{d,h} + \sum_{h=23}^{24} wp_{d,h} \cdot y_{d,h})}{\sum_{d=1}^{365} (\sum_{h=1}^{6} y_{d,h} + \sum_{h=23}^{24} y_{d,h})} \tag{C.5}$$

$$ep^{tou3,l2} = \frac{\sum_{d=1}^{365}(\sum_{h=7}^{16} wp_{d,h} \cdot y_{d,h} + \sum_{h=20}^{22} wp_{d,h} \cdot y_{d,h})}{\sum_{d=1}^{365}(\sum_{h=7}^{16} y_{d,h} + \sum_{h=20}^{22} y_{d,h})} \tag{C.6}$$

$$ep^{tou3,l3} = \frac{\sum_{d=1}^{365} \sum_{h=17}^{20} wp_{d,h} \cdot y_{d,h}}{\sum_{d=1}^{365} \sum_{h=17}^{20} y_{d,h}} \tag{C.7}$$

$$ep_t^{tou3} = \begin{cases} ep^{tou3,l1}, & \text{if } t \in [24k+1,\ 24k+6] \\ & \bigcup [24k+23,\ 24k+24] \\ & \text{with } k \in [0,364] \\ ep^{tou3,l2}, & \text{if } t \in [24k+7,\ 24k+16] \\ & \bigcup [24k+21,\ 24k+22] \\ & \text{with } k \in [0,364] \\ ep^{tou3,l3}, & \text{if } t \in [24k+17,\ 24k+21] \\ & \text{with } k \in [0,364] \end{cases} \tag{C.8}$$

The last tariff to determine is the RTP tariff ep_t^{rtp}. Here, wholesale prices at every hour of the year wp_t are directly passed on to the consumers, as shown in Equation C.9.

$$ep_t^{rtp} = wp_t, \quad t \in [1, 8760] \tag{C.9}$$

C.3 Heating

The total heating demand of households can be estimated based on the number of inhabitants and the size of the living space. Since this data is not included in the original electricity consumption data set, it is estimated based on the households' annual electricity consumption in the first year, divided by the average electricity consumption in the UK (Topping, 2021; Clark, 2021). By multiplying the calculated number of inhabitants with the average apartment size per person in London (33 m^2), the living space of each household is determined (Coshand and Gleeson, 2020). Taking the average annual heating demand per square meter of 133 kWh/m^{2}a into account, the annual heating capacity required is determined (Marcus, 2021). For water heat demand, the average water consumption of 40 liters per person and day multiplied by the energy needed to heat it up to 40°C (von der Lühe, 2018).

The daily demand for hot water is assumed to be static over the year. The heating demand for space heating needs to be distributed over time. For this, we take advantage of historical, hourly resolved, temperature data from London in 2012 and 2013 (kaggle, 2019). We assume that space heat is only produced when temperatures are below the heating limit with a daily average temperature of 12°C (in line with Recknagel et al. (2006)). This leads to 214 heating days in the first year and 202 heating days in the second year. The space heat demand is then equally distributed over the heating days.

C.4 Mobility

For this study, we use mobility data from the German Mobility Panel (Ecke et al., 2019). It includes detailed driving profiles of private households in Germany in everyday life during an ordinary week. The data collection includes various data of which we use the ID, means of transportation, day of the week, departure time, distance travelled, arrival time, and trip purpose. We only consider trips for which a car is used as means of transportation.

From the panel's extensive data collection, a commuter and a non-commuter driving profile is randomly assigned to each electricity consumption profile, which creates two synthetic customers for each consumption profile and enables a comparison of the two characteristics. A driving profile is considered to be a commuter profile if the workplace is visited at least four times a week. We only consider profiles for which the parking time of the car at home is always long enough to recharge the car sufficiently to complete the subsequent trips until the car returns home. Finally, the mobility profile is extended to the two year time frame of the case study, by repeating the driving profiles.

APPENDIX D

PROBABILISTIC FORECASTING BENCHMARK RESULTS

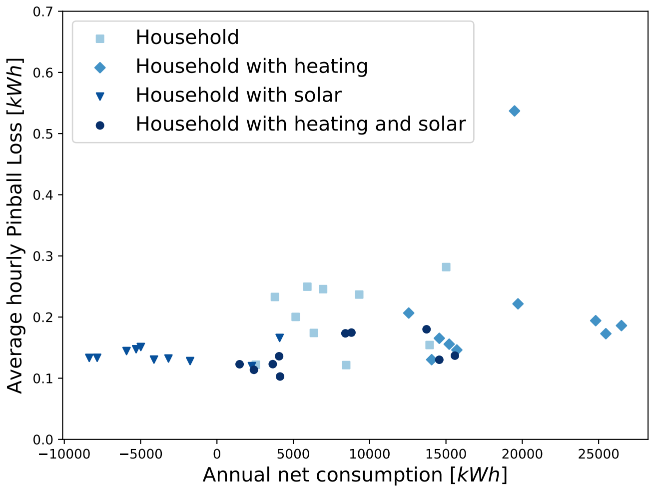


Figure A.1.: Net load and QLSTM pinball loss

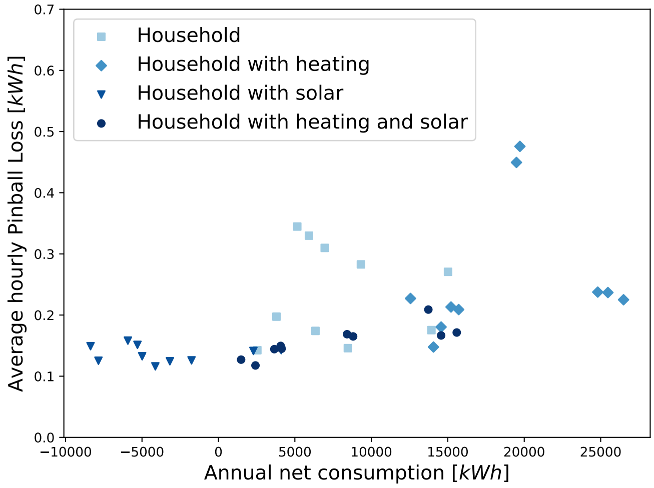


Figure A.2.: Net load and QREGNN pinball loss

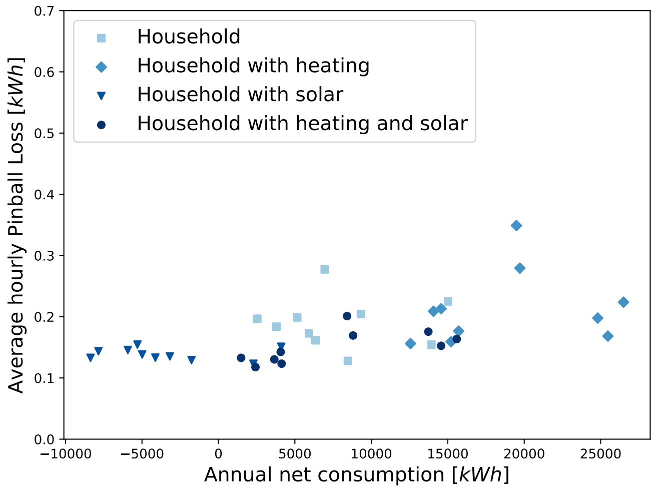


Figure A.3.: Net load and QLSTM_noWeather pinball loss

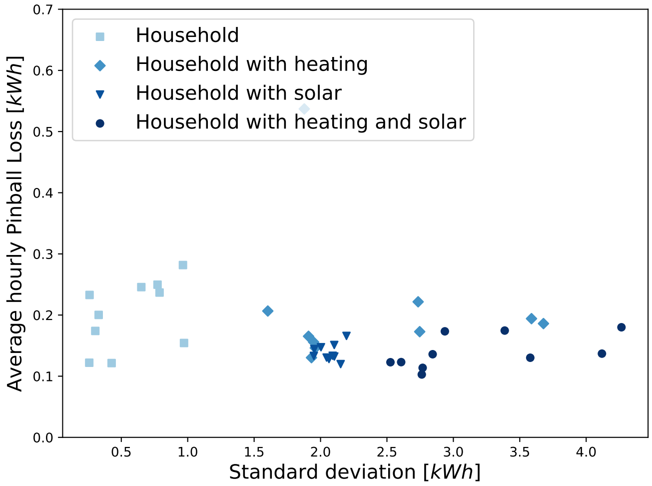


Figure A.4.: Standard deviation and QLSTM pinball loss

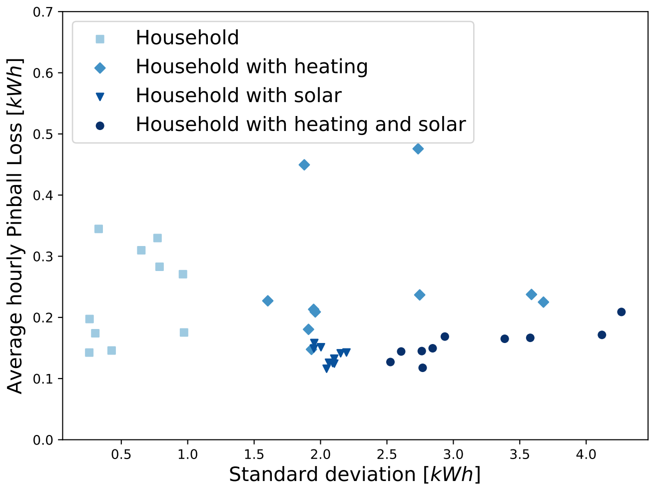


Figure A.5.: Standard deviation and QREGNN pinball loss

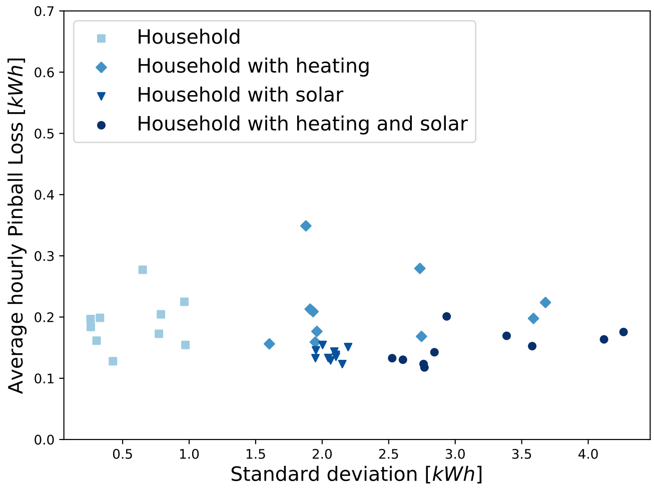


Figure A.6.: Standard deviation and QLSTM_noWeather pinball loss

APPENDIX E

HYDROGEN DEMAND DATA

E.1 Steel

To identify all steel plants with potential for hydrogen use in 2030, we use the statistical report of the steel industry (WV Stahl, 2020). Looking at future hydrogen demand, only those 70 % of steel producers who manufacture via the blast furnace route are relevant, as large quantities of CO_2 are emitted here and can be avoided by switching to the direct reduction route. In addition, the ArcelorMittal plant in Hamburg is included, as it already uses a direct reduction approach (Hölling et al., 2017). Table 9.4 lists the eight identified steel production sites.

The production volumes and relative shares of primary and secondary steel in Germany have been approximately constant since 2012 (WV Stahl, 2020). Therefore, and in line with Hebling et al. (2019), we use past production volume and distribution as 2030 estimates. In particular, we use 2017 values, as only those are available in (WV Stahl, 2020). However, it can be assumed that not all steel producers will switch to direct reduction by 2030, due to various reasons. For instance, the switch is associated with high investment costs, is technically demanding (IKTS, 2020), and comes with new uncertainties like future hydrogen costs (Agora Energiewende and Wuppertal Institut, 2019). Correspondingly, steel producers are planning individual solutions for medium-term CO_2 emission reduction to achieve reduction goals. Therefore, all relevant plants must be analyzed individually, via online research and direct communication with the relevant companies.

ArcelorMittal Hamburg has been operating a direct reduction plant since the mid-1970s (Hölling et al., 2017). The reduction gas used today consists of about 60 % hydrogen (ArcelorMittal, 2017). By 2030, steel production is planned to be completely CO_2-neutral (ArcelorMittal, 2020a). Accordingly, we assume that there will be a complete switch to the direct reduction route with 100 % hydrogen input by 2030. For the direct reduction route, we assume the specific hydrogen demand factor $80kg_{H_2}/t_{steel}$, based on Michalski et al. (2019). The hydrogen demand of ArcelorMittal Hamburg for the year 2030 is estimated with Equation E.1.

$$HD = Output_{t_{Steel}} \cdot specificDemandFactor \cdot 33.33kWh_{H_2}/kg_{H_2} \tag{E.1}$$

ArcelorMittal Eisenhüttenstadt and ArcelorMittal Duisburg have not publicly announced any plans to use hydrogen until 2030, but it has been indicated that long-term adoption of hydrogen for the former plant will depend on the results of current pilot projects of the ArcelorMittal group (ArcelorMittal, 2020b). Therefore, we assume that these plants do not have any hydrogen demand in 2030.

ArcelorMittal Bremen is focusing on the use of hydrogen via the blast furnace route to achieve the medium-term goals. However, the company already plans to construct an electrolyser on-site (swb, 2020) that will be sufficient to fully meet the hydrogen demand in 2030. Thus, the plant does not have any net demand for hydrogen.

ROGESA, a subsidiary of Dillinger and Saarstahl, produces pig iron, which is supplied to Dillinger and Saarstahl for the subsequent crude steel production (Dillinger, 2016). Therefore, Dillinger and Saarstahl are considered collectively for further calculations. ROGESA operates two blast furnaces and plans to optimise both by blowing in hydrogen as a reducing agent in order to achieve a reduction in CO_2 emissions (Dillinger, 2019). According to a step-by-step plan of the Saarland-based steel industry, both blast furnaces are to remain in operation until 2031 (Warscheid, 2020a). In addition, an electric furnace and a direct reduction plant are to be built, which will initially only use natural gas to produce directly reduced iron from iron ore (Warscheid, 2020a). Therefore, we assume that by 2030, both blast furnaces will use the maximum amount of hydrogen. Both blast furnaces are technically able to use a maximum of approximately 3,700 kg_{H_2}/h (Warscheid, 2020b; ROGESA, 2016). Thus, the hydrogen demand of ROGESA (Dillinger and Saarstahl) for the year 2030 is estimated to be 2.1606 TWh_{H_2}, based on Equation E.2. [35]

$$HD = 2 \cdot 3700 kg_{H_2}/h \cdot 8760 h \cdot 33.33 kWh_{H_2}/kg_{H_2} \tag{E.2}$$

Hüttenwerke Krupp Mannesmann (HKM) is owned 50 % by Thyssenkrupp Steel Europe AG, 30 % by Salzgitter Mannesmann GmbH and 20 % by Vallourec Tubes S.A.S (HKM, 2020). Regarding the use of hydrogen in production, no press reports were found. Consequently, it is assumed that due to the structure of the company, no hydrogen will be used until 2030, as the shareholders might primarily concentrate on their own production facilities and their optimisation.

Salzgitter is pursuing a gradual conversion to hydrogen-based steel production via the direct reduction/electric arc furnace route. In the first stage of expansion, a direct reduction plant and an electric arc furnace will be built (Redenius, 2020a). This expansion stage will lead to a hydrogen use of 81,332 Nm^3/h and a specific hydrogen demand factor of 12.27 kg_{H_2}/t_{steel} (Redenius, 2020b) for the overall plant output. Thus, the hydrogen demand for 2030 can be calculated with equation E.1.

Thyssenkrupp plans to replace two blast furnaces with two direct reduction plants, and to optimize one blast furnace by blowing in hydrogen until 2030 (Thyssenkrupp, 2020a). Current estimations indicate that around 200,000 tons of hydrogen per year will be needed from 2030. A share of this will be supplied through a long-term contract with RWE, from a 100 MW electrolyzer capable of supplying 1.7 tons of hydrogen per hour (Thyssenkrupp, 2020b). This supply is deducted from the total demand in order to calculate the hydrogen net demand for 2030 as shown in Equation E.3.

$$HD = (200,000,000 kg_{H_2} - 1,700 kg_{H_2}/h \cdot 8,760 h) \cdot 33.33 kWh_{H_2}/kg_{H_2} \tag{E.3}$$

[35] To validate the results, we also estimate the demand with Equation E.1, which returns 2.0668 TWh_{H_2} and thus confirms the calculations. For all further calculations, we use 2.1606 TWh_{H_2} as demand for the Dillinger and Saarstahl steel plants.

E.2 Ammonia

The ideal specific hydrogen demand for ammonia synthesis is 3 moles of H_2 for 2 moles of NH_3 (Hermann et al., 2014), or 177.55 kg_{H2} per ton of ammonia.

We acquire a list of all ammonia producers in Germany from the Industrial Association Agrar (IVA, 2018). The production volumes of ammonia in Germany have been approximately constant since 2012 (VCI, 2020). While, to the best of our knowledge, no information on site-specific current ammonia production is publicly available, we identify site-specific production capacities based on online research Peters and Thumann (2016); Bezirksregierung Köln (2017) and direct communication with the companies. The sum of these capacities (2,955,000 t/a) is somewhat higher than the current total ammonia production (2,415,327 in 2019). However, global ammonia demand is assumed to increase by 2030 (Hebling et al., 2019; International Energy Agency, 2019a). Therefore, in the following, the production capacities are assumed as basis for the site-specific hydrogen demand estimation.

With the assumptions made above, the site-specific demand can be estimated with Equation E.4.

$$HD = t_{Ammonia} \cdot 177.55 kg/t_{Ammonia} \cdot 33.33 kWh_{H_2}/kg_{H_2} \tag{E.4}$$

E.3 Methanol

The specific hydrogen demand is estimated as 2 moles of H_2 for 1 mole of CH_3OH (Hofbauer et al., 2016), or 188.73 kg_{H2} per ton of methanol. This is consistent with the assumptions of Bazzanella and Ausfelder (2017) and Michalski et al. (2019). Currently, there are five relevant methanol plants in Germany (Fröhlich et al., 2019). However, one of them has terminated production and is being liquidated, and therefore is disregarded for 2030.

In the next step, production capacities of the individual plants are identified (Fleiter et al., 2013; Jendrischik, 2020; BP, 2019). The sum of current production of 1,398,146 t/a (VCI, 2020) is lower than the total production capacity of 1,865,000 t/a. However, production has been rising in recent years, and global methanol demand is assumed to increase by 2030 (Hebling et al., 2019; International Energy Agency, 2019a). Correspondingly, as with the hydrogen estimate for ammonia, the production capacity is used as basis for further calculations.

With the assumptions made above, the site-specific demand can be estimated with Equation E.5.

$$HD = t_{Methanol} \cdot 188.73kg/t_{Methanol} \cdot 33.33kWh_{H_2}/kg_{H_2} \tag{E.5}$$

E.4 Refineries

We use the list of all refineries and their output capacities from the German Petroleum Industry Association (MWV, 2020). Mineral oil consumption will decrease by varying degrees by 2030, depending on assumptions about the demand for liquid fuels (Michalski et al., 2019). Correspondingly, the current production volume of 87,013,000 tons is distributed across the sites in proportion to their processing capacity. Then, following Prognos AG (2020a), the assumption is made that the demand for mineral oil will decrease by about 20 % until 2030.

The specific hydrogen net demand is assumed to be approximately 100 $m^3_{H_2}$ per ton crude oil, based on Schweer et al. (2002). Thus, the site-specific hydrogen demand for refineries can be estimated with Equation E.6.

$$HD = t_{Oil,pq,2030} \cdot 100m^3/t_{Oil,pq,2030} \cdot 0,0841 \cdot kWh_{H_2}/kg_{H_2} \cdot 22\% \tag{E.6}$$

APPENDIX F

CONVERSION FACTORS

Table A.1.: Numeric values and conversion factors for H_2

Lower heating value of hydrogen	33.33 kWh/kg
Conversion factor kg in m^3	11.89
Conversion factor m^3 in kg	0.0841

APPENDIX G

SENSITIVITY SCENARIOS

There is one sensitivity scenario for the hydrogen demand and one for the electricity generation. For the sensitivity scenarios, it is assumed that a hydrogen delivery truck has a consumption of 6.75 kg per 100 kilometers and investment costs of 174,000 EUR (Gnann and et al., 2017).

Since it is highly disputed and unclear if there will be relevant numbers of fuel cell passenger cars in Germany in 2030 (He et al., 2021; Insider, 2020; Li et al., 2016; Morrison et al., 2018), we calculate an alternative scenario without hydrogen fueled cars.

Neglecting hydrogen cars reduces the electricity demand caused by hydrogen production from 72.5 to 68.2 TWh/year. Since hydrogen car refueling stations would be distributed across the country, neglecting them leads to a more concentrated demand a fewer (industry) locations. Consequently, under the uniform tariff, hydrogen integration without hydrogen cars increases redispatch costs to 7,282.38 MEUR/year (Flat, static operation), compared to 7,253.56 MEUR/year in the case with hydrogen cars. Under the nodal tariff, redispatch costs decrease to 5,209.15 MEUR/year (Flat, static operation), compared to the benchmark without hydrogen, but are higher than the 5,100.84 MEUR/year in the case with hydrogen cars. Since in the nodal tariff case, hydrogen is produced at low cost nodes, lower overall hydrogen demand leads to lower volumes of avoided redispatch.

As wind energy offers greater potential in northern Germany than southern Germany, the majority of wind generation capacity is located in the North, leading to spatial imbalances of generation and demand. To address this, the Federal Ministry for Economic Affairs and Energy introduced the so-called *Southern Quota* in the renewable energy act of 2021. The quota reorganizes the distribution of subsidies for new wind energy projects. A particular percentage of the financial subsidies is exclusively available to the construction projects in southern counties (Bundesministerium für Wirtschaft und Energie, 2021). The percentage of the *Southern Quota* for onshore wind turbines is set to 15% for 2021 to 2023 and to 20% for 2024 and later. A list of the southern counties is shown in Bundesministerium für Wirtschaft und Energie (2021). We calculate an alternative scenario that takes this quota into account for all newly added onshore wind generation capacity until 2030.

Taking into account the *Southern Quota* affects the geographical distribution of wind energy, and thus nodal electricity prices. These in turn impact the optimal locations of electrolyzers and the integration effects. The baseline redispatch costs without hydrogen are 5,622.82 MEUR/year (Flat, static operation). This is less than the 6,163.96 MEUR/year in the case without the quota. Integrating hydrogen under uniform tariffs increases redispatch costs to 6,648.89 MEUR/year (Flat, static operation), which is less than the 7,253.56 MEUR/year in the case without the quota. Integrating hydrogen under nodal tariffs decreases redispatch costs to 4,701.27 MEUR/year, which is again less than the 4,915.41 MEUR/MWh without the quota. This shows that in addition to the positive effects of spatial signals for new electricity demand (i.e. nodal tariffs for electrolyzers) it is also beneficial for the electricity system to have spatial signals for new generation (i.e. regional quotas for wind turbines).

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