Transition Technologies for Electrification and Optimisation of Bus Transport Systems

The C40-city of Curitiba in Brazil

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ABSTRACT

The topical issue of climate change has increasingly become important as scenarios indicate an increase of 2.5–7.8°C in the global mean temperature by the end of this century, if no greenhouse gas emissions are reduced. The transport sector depends strongly on fossil fuels and has been therefore considered as one key sector concerning climate change mitigation. In this regard, a key role is played by cities, since progressing urbanisation will presumably lead to a higher demand for urban transport.

This doctoral thesis addresses the transition phase of public bus transport systems by exploring electrification as a vector for decarbonisation. The C40-city of Curitiba in Southern Brazil is used as a case study. The research is of explorative and empirical nature. Quantitative research methods are applied to compare bus technologies as well as new optimisation models and planning tools are developed to support data analytics and research in the areas of simulation, optimisation and (long-term) planning of energy and transport systems at different levels of consideration.

The results from the comparison of different buses show large potentials to save energy and reduce emissions during the operation phase, for example, when using hybrid-electric or plug-in hybrid-electric buses instead of conventional buses. Moreover, energy savings in the operation phase also imply avoidance of fuel production and supply. Additionally, electrified buses can also reduce operational uncertainty caused by varying driving cycles and fluctuating fuel prices concerning an absolute variation of both energy use and fuel cost in the operation phase.

A real-time optimisation model was developed, and its concept tested to estimate potentials for energy savings and all-electric operation from the operational optimisation of a plug-in hybrid-electric bus fleet. Different management strategies were simulated concerning the charging schedule and all-electric operation of the bus fleet. While energy savings can be significantly increased through a structural change towards more electrified buses, a large potential to increase the total all-electric operation of the bus fleet was estimated through operational optimisation. Consequently, both a structural change and operational optimisation should be jointly applied to maximise the benefits gained from electrification in a bus transport system.

The software system OSeMOSYS-PuLP was developed for empirical deterministic-stochastic modelling based on the OSeMOSYS modelling framework, which enables the use of a Monte Carlo simulation. The open source design of the tool shall enhance transparency and trustworthiness in studies. It is transferable to many cases and enables analysts and researchers to generate new sets of conclusions together with associated probability distributions considering the use of real-world datasets, e.g. from open data initiatives as the one in Curitiba.

In summary, the research findings, applied methods and developed tools can be used to support and inform analysts and decision-makers in the area of transport and energy systems planning in data-driven decision-making processes to develop and assess different technological options and strategies at different levels while considering associated uncertainties.

Keywords
Bus transport system; C40; Decarbonization; Electrification; GHG; Optimization; OSeMOSYS-PuLP; Plug-in hybrid-electric; Systems analysis; Transformation
SAMMANFATTNING

Den aktuella frågan om klimatförändringar har blivit allt viktigare eftersom scenarier indikerar en ökning med 2,5–7,8°C i den globala medeltemperaturen i slutet av detta århundrade, om inga utsläpp av växthusgaser minskar. Transportsektorn är starkt beroende av fossila bränslen och har därför betrakts som en nyckelsektor när det gäller att minska klimatförändringarna. I detta avseende spelar städer en nyckelroll, eftersom en framtida urbanisering förmodligen kommer att leda till en ökad efterfrågan på stadstrafik.


Resultaten från jämförelsen av olika bussar visar stora möjligheter att spara energi och minska utsläppen under driftsfasen, till exempel när man använder hybrid-elektriska eller laddhybrid-elektriska bussar istället för konventionella bussar. Dessutom innebär energibesparingar i driftsfasen också undvikande av bränsleproduktion och -försörjning. Dessutom kan elektrifierade bussar också minska driftsåkertider orsakad av varierande körcyklar och fluktuerande bränslepriser beträffande en variation av både energianvändning och bränslekostnader i driftsfasen.

En realtidsoptimeringsmodell utvecklades och dess koncept testades för att uppskatta potentialen för energibesparingar och helelektrisk drift från driftsplanering av en laddhybrid-elektrisk bussflotta. Olika förvaltningsstrategier simuleras beträffande laddnings schemat och elektrisk drift av bussflottan. Medan energibesparingar kan ökas betydligt genom en strukturerande förändring mot mer elektrifierade bussar, uppskattades en stor potential för att öka den totala elektriska driften av bussflottan genom driftsplanering. Följaktligen bör både en strukturell förändring och driftsplanering tillämpas gemensamt för att maximera fördelarna från elektrifiering i ett busstransportsystem.

Programvarusystemet OSeMOSYS-PuLP utvecklades för empirisk deterministisk-stokastisk modellering baserat på OSeMOSYS-modelleringsramverket, vilket möjliggör användning av en Monte Carlo simulering. Den öppna källkods-designen av verktyget ska öka insynen och pålitligheten i studier. Det kan överföras till många fall och gör det möjligt för analytiker och forskare att generera nya slutsatser tillsammans med tillhörande sannolikhetsfördelningar med tanke på användningen av verklig data, t.ex. från öppna datainitiativ som i Curitiba.

Sammanfattningsvis kan forskningsresultaten, tillämpade metoder och utvecklade verktyg användas för att stödja och informera analytiker och beslutsfattare inom området transport och energisystemplanering i datadrivna beslutsprocesser för att utveckla och utvärdera olika tekniska alternativ och strategier på olika nivåer med hänsyn till tillhörande osäkerheter.

Nyckelord
Bussstransportsystem; C40; Elektrifiering; Koldioxidminskning; Laddhybrid; Optimering; OSeMOSYS-PuLP; Systemanalys; Transformation; Växthusgaser
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Dennis Dreier
Stockholm, Sweden, 2020
PUBLICATIONS

This doctoral thesis compiles research results of four scientific papers:

**Paper I**


**Paper II**


**Paper III**


**Paper IV**


**Source code repository**

OSeMOSYS-PuLP: https://github.com/OSeMOSYS/OSeMOSYS_PuLP

**Declaration of the thesis author’s contributions**

The publications were developed in collaboration. The thesis author (D.D.) declares his contribution in the following using the terms of the CRediT by (CASRAI, 2019):


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**Transition Technologies for Electrification and Optimisation of Bus Transport Systems**

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1 **INTRODUCTION**

This introductory chapter starts with presenting the topical challenges and overarching objective of the research in this doctoral thesis. Based on that, the state-of-the-arts literature is reviewed, knowledge gaps are pointed out, and research questions are derived. Accordingly, scope and relevance of the thesis are elaborated. The chapter ends with presenting an outline of the thesis over the remaining chapters. Note: A list of abbreviations and units, and a glossary for technical terms are provided in the Appendix.

1.1 **TOPICAL CHALLENGES**

The topical issue of climate change has become increasingly important as scenarios indicate an increase of 2.5–7.8°C in the global mean temperature by the end of this century, if no greenhouse gas (GHG) emissions are reduced (IPCC, 2015). Current research predicts that this will very likely have grave consequences, such as substantial reduction in biodiversity (Warren et al., 2013), disruption of the ecosystem’s structure, services and functions (Gaston and Fuller, 2008), river flooding (Alfieri et al., 2017), welfare losses (Dottori et al., 2018), etc. Obviously, the complexity of global warming poses a severe threat to the earth and us — humankind. Hence, countries must jointly act to first stabilise and then reduce anthropogenic GHG emissions for the mitigation of potential damages. In December 2015, a historical agreement was made at the Conference of the Parties (COP) 21 — the Paris Agreement — that goal it is to limit the global mean temperature rise to well below 2°C compared to pre-industrial levels — referred to as the climate target (UNFCCC, 2015).

One key sector is the transport sector that accounts for 27% of the global total final energy use and emits 23% of the global energy-related carbon dioxide (CO₂) emissions (IEA, 2017c). Furthermore, CO₂ emissions were rising by 2.5% annually over the period 2010–2015 (IEA, 2017c). In this respect, road transport is particularly important, as it mainly depends on fossil oil products and accounts for 93% of the latter’s final energy use (IEA, 2018). Besides, road transport is the largest polluter among all transport modes, e.g. in the case of the European Union, this subsector accounts for 73% of all transport-related GHG emissions (European Commission, 2016b). In addition to its already tremendous energy use and emissions, projections...
foresee a doubling of the road transport sector’s energy use by 2050 (IPCC, 2015). Opposite to this scenario, some estimations state a reduction potential of 15–40% by 2050 (IPCC, 2015).

In the case of Brazil, the transport sector accounts for 37% of the country’s total final energy use (IEA, 2017b). The largest energy resources in the country’s transport sector are oil products, accounting for 77% of the sector’s total final energy use, followed by 20% biofuels and the remainder for natural gas and electricity (IEA, 2017b). Furthermore, the transport sector accounts for 48% of Brazil’s CO₂ emissions released from fuel combustion (IEA, 2017a).

Meanwhile, Brazil intends to reduce GHG emissions by 37% in 2025 compared to 2005 levels according to their contribution to the Paris Agreement (Federative Republic of Brazil, 2015). Moreover, Brazil intends to “further promote efficiency measures, and improve infrastructure for transport and public transportation in urban areas.” (Federative Republic of Brazil, 2015).

In Brazil as well as globally, a key role in the trend to reduce energy use and GHG emissions is played by cities, since urbanisation progresses (UN Department of Economic and Social Affairs, 2019) and will presumably lead to a higher demand for urban mobility. Nowadays, cities emit up to 70% of the global GHG emissions according to both consumption-based and production-based accounting methods (UN-Habitat, 2011). Thus, the reduction of fossil fuel use and the consequent reduced amount of GHG emissions from urban transport systems is essential with respect to the climate target, i.e. a decarbonisation of transport systems in cities. In addition to gaseous emissions, the emission of noise has got more attention lately. Noise in urban areas is mainly caused by traffic, e.g. as shown in case studies for New York City and Hong Kong (McAlexander et al., 2015; Ross et al., 2011; To et al., 2002), and furthermore, it is considered as one of the most severe health threats to humans (European Commission, 2017a; WHO, 2012).

Meanwhile, cities have started to form networks, in which they coordinate and address jointly the previously mentioned issues of global and local emissions. One network is the C40 Cities Climate Leadership Group (C40): “C40 is a network of the world’s megacities committed to addressing climate change. C40 supports cities to collaborate effectively, share knowledge and drive meaningful, measurable and sustainable action on climate change.” (C40, 2019c). The C40 consists of 94 cities, in which more than 650 million people live that produce 25% of the global gross domestic product (C40, 2019c). In addition to megacities, a couple of other cities were invited to become C40 members. Those cities are classed as innovator cities and show a clear leadership towards environmental sustainability and climate change mitigation. One of the innovator cities is the city of Curitiba in the South Region of Brazil that is used as a case study in this thesis. Curitiba and the remaining C40 cities are shown on the world map in Figure 1.

Curitiba has been internationally recognised as a leader in innovative urban transportation, especially considering that the world-famous bus rapid transit (BRT) concept was created in this city in 1970s. The BRT concept is a cost-effective bus-based transit system that provides fast and comfortable transport service at similar passenger carrying capacity (PCC) and convenience levels as metro systems (ITDP, 2018). BRT features are exclusive bus lanes, and their alignment to the centre of the road, off-board fare collection, platform level boarding and prohibition of turning on/over BRT lanes for other traffic (ITDP, 2018). The combined benefits are a faster and more frequent operation of buses while avoiding delays due to mixed traffic congestion or passenger queuing for on-board fare payments as in regular bus transport systems. The capital cost for a BRT system can be 4–20 times lower than for a light rail transit system, and 10–100 times lower than for a metro system (Wright and Hook, 2007). This noteworthy cost effectiveness makes the BRT concept an attractive option for cities in both developed and developing countries (Hensher and Golob, 2008; Hensher and Mulley, 2015; Zhang, 2009). As a result of these distinct
operational and cost advantages, BRT systems have been implemented in 171 cities globally, and are used by almost 34 million passengers per day now — with the largest share in Latin America (BRTdata, 2019b). The aggregated distance of BRT kilometres built worldwide amounts to 5145 kilometres (BRTdata, 2019b). Interestingly, the most development has been done as of the year 2000 in terms of new implementations and distance expansions (BRTdata, 2018a; Hidalgo and Gutiérrez, 2013). This development trend highlights the increasing interest and need for this transport concept in cities, e.g. those cities mentioned by (Hensher and Li, 2012b; Hensher and Li, 2012a; Heres et al., 2014). Noteworthy, the BRT concept is also taken into consideration as an important measure for decarbonisation in the case of Brazil (La Rovere et al., 2015).

Bus transport systems, to which the BRT concept belongs to as a subset, are the primary form of public transport in the world (UTIP, 2014). Similarly in the case of Curitiba, where the ridership of the city’s public bus transport system amounts to 1.37 million trips per day (URBS, 2018e), which gives a total mileage by the bus fleet of 300 000 km per day on average (URBS, 2018d). Considering that the population of Curitiba amounts to 1.9 million inhabitants (IBGE, 2017), the ridership implies the high importance of the bus transport system for passenger transport in the city. This indication is supported by statistics according to (BRTdata, 2019a), stating that the modal split in Curitiba amounts to 46% for public transport, 26% for private transport and 28% non-motorised transport modes.

Considering that a bus only emits a quarter of the CO₂ emissions per passenger-kilometre of a car (UTIP, 2014), a modal shift from a large fleet of private cars to a smaller fleet of buses is desirable. However, this measure will presumably result in more passengers that must be transported. Thus, either more or larger buses will be needed to meet the increased transport demand. Based on this scenario, a modal shift will presumably cause more GHG emissions from a bus fleet and therefore, technical enhancements or replacements of existing buses will be also required to reduce further GHG emissions concerning the climate target.

![Figure 1: Geographical locations of the C40 cities (C40, 2019c; Qlik, 2019; OpenStreetMap contributors, 2019)](image-url)
Curitiba and 25 other C40 cities as well as 11 non-C40 supporting cities and regions have signed a commitment since its first announcement at the C40 Latin American Mayors Forum in 2015 — the C40 Cities Clean Bus Declaration of Intent (C40, 2015b). The plan provides that more than 40 000 clean buses shall be deployed by 2020. This declaration is considered as the first step of city governments and bus manufacturers to achieve decarbonised urban transport with the aim to achieve zero GHG emissions in the long-term. The declaration describes clean buses as “low and ultimately zero emission buses” (C40, 2015b). Although this term leaves room for interpretation, possible examples could be advanced buses that use to some extent electricity for propulsion, such as hybrid-electric buses, plug-in hybrid-electric buses, battery-electric buses and fuel cell buses. And these types of buses are also already available on the market. Subsequent to the C40 Cities Clean Bus Declaration of Intent (C40, 2015b), the Fossil Fuel Free Streets Declaration was signed; first by twelve cities in 2017 (C40, 2017), and in total by 26 cities by now (C40, 2019a). The latter declaration reinforces the C40’s ambitions and states the goal to transition into decarbonised transport by “Procuring, with our partners, only zero-emission buses from 2025; and ensuring a major area of our city is zero emission by 2030.” (C40, 2017).

The introduction of new technologies is usually not a straightforward process and requires the consideration of potential operational issues. The current status of operating bus fleets is that those consist predominantly of conventional buses (BRTdata, 2018b). A conventional bus uses an internal combustion engine for propulsion and is often fuelled with petroleum diesel (BRTdata, 2018b). The amount of fuel in the fuel tank is usually enough for continual driving of 300 km without any refuelling (Mahmoud et al., 2016). In comparison, the all-electric drive capabilities of electrified buses often lasts for 7–200 km when starting with a fully charged battery that needs to be recharged then (Volvo Group UK, 2017; Mahmoud et al., 2016; Stokes and Poger, 2013). The all-electric range is a crucial parameter and can raise the issue of range anxiety — especially for battery-electric buses. In contrast, plug-in hybrid-electric buses employ, in addition to an electric motor, an internal combustion engine as a range extender. Thus, this type of bus can still operate when the battery is completely depleted by using diesel or another type of fuel. However, the associated energetic and environmental benefits, such as energy savings and GHG emissions reduction as well as silent operation (Borén et al., 2016), are still lost then. Based on that, the aim should be to strive for as much all-electric driving as possible. Especially in the case of Brazil, where renewable energy sources contribute to 79% of the country’s electricity mix — whereof hydropower generates the largest share with 62% (IEA, 2017a). Otherwise, no improvements would be the result, since a plug-in hybrid-electric bus would use its internal combustion engine just as a conventional bus. One solution could be the installation of a larger battery in terms of nominal capacity. However, this would also increase the capital cost of a bus. For example, considering that the battery accounts for 23% of the capital costs of a battery-electric bus (Ding et al., 2015; Olsson et al., 2016), a larger battery would considerably increase the price tag. In comparison, a widespread implementation of charging infrastructure represents another solution to still overcome the obstacle of range anxiety. With this, plug-in hybrid-electric and battery-electric buses can be recharged during operation, e.g. using the concept of opportunity charging with deployment of fast charging stations. Furthermore, opportunity charging can be conducted at bus stations. Here, the dwell time of a bus can be simultaneously used to recharge the battery while passengers embark and disembark. Nevertheless, heavy investments would be still required to transform bus transport systems. Consequently, the bus technologies of hybrid-electric and plug-in hybrid-electric buses can be considered as transition technologies, since they do not completely rely on charging infrastructure, but can still save energy, cut GHG emissions and reduce noise.
This makes them interesting for cities as a starting point in the transformation process of their urban transport systems with the aim for decarbonisation. Taking into consideration the current early stages or even non-existing transformations of bus transport system in cities, both hybrid-electric and plug-in hybrid-electric buses represents viable options to start with.

The redesign of bus transport systems is not limited to the introduction of advanced (electrified) buses or deployment of charging infrastructure per se. The planning of a system’s operation can be also included to ensure a reliable transport service without any delays or gridlocks. Additionally, other strategies could be considered. For example, once two or more plug-in hybrid-electric buses are operated, the following situation can come up that both buses arrive simultaneously at the same charging station and must be charged. In this case, a decision is needed which bus to prioritise for charging and how long that bus should be charged. Certainly, one solution is a prioritisation based on the principle first come, first served, i.e. the bus that arrives first is charged first, while the remaining buses are not charged or need to wait until the charging process of the first bus is completed. However, another aim could be to maximise the total all-electric operation of all buses together. This might lead to the situation, that the bus that arrives second is prioritised for charging based on the prediction that the total all-electric operation of all buses would be larger than if the first bus was charged and the remaining buses then. Moreover, another operational strategy could be to plan when to drive all-electric rather than simply driving all-electric only because electricity is available in the battery. Based on those considerations, different decisions could be made concerning the charging schedule and all-electric operation of a plug-in hybrid-electric bus fleet. Those strategies and resulting decisions can be defined in management strategies.

Another challenge is the long-term planning and transformation of a system. The introduction of new bus technologies in a bus transport system also requires the provision of new fuels, such as electricity. The transformation is a cost and time-intensive process that goal it is to improve current conditions and solve existing problems, e.g. reduction of GHG emissions, local air pollution and noise in the case of conventional buses. Eventually, decisions must be found to agree on the transformation of a system and associated goals. In this respect, the development of long-term planning scenarios for transport and/or energy systems has been a valuable tool to evaluate advantages and disadvantages associated with a transformation. Additionally, models represent a cost-efficient and safe approach to test ideas and strategies, and to quantify their impacts on economy, environment and/or society (Subramanian et al., 2018). Those models rely on representative input data collected from the real world. However, that data also contains associated uncertainties and randomness from the real world. Thus, modelling frameworks should be designed in such a way that those can incorporated uncertainties and evaluate their impact on strategies, insights and conclusions.

Overall, the transformation of a bus transport system must consider a variety of aspects at different levels, such as the bus technology level, the bus fleet management level, and the long-term system planning level. The research in this thesis is of explorative and empirical nature. Quantitative research methods are applied to compare bus technologies as well as new models and tools are developed to extend research possibilities concerning the simulation, optimisation and (long-term) planning of energy and transport systems. The research findings, models and tools are used to analyse opportunities, drawbacks and uncertainties associated with the transformation of bus transport systems. As the C40 considers itself as a data-driven organisation (C40, 2015a), this thesis is also in line with the C40 network’s approach as well as contributes to other initiatives concerned with transforming bus transport systems with the goal of decarbonisation to reduce their climate impact.
1.2 Objective

The overarching objective of this doctoral thesis is to support and quantify opportunities in the transition phase of bus transport systems from operating conventional buses to using electrified buses by exploring electrification as a vector for decarbonisation. The C40-city of Curitiba in Brazil is used as a case study. Locally relevant recommendations are derived from the case study and ought to be also transferable as recommendations to other C40 and non-C40 cities globally.

The empirical findings and methodological contributions of this thesis intend to mainly contribute to the following Sustainable Development Goals (SDGs) set out by the Agenda 2030 development programme of the United Nations (UN, 2018) and in particular to the following associated targets:

SDG 3: Good health and well-being (Targets 3.9 and 3.9.1); SDG 7: Affordable and clean energy (Target 7.3); SDG 11: Sustainable cities and communities (Targets 11.2, 11.3 and 11.6.2); SDG 13: Climate action (Targets 13.2 and 13.2.1). Note: descriptions of targets are provided in the Appendix.

Accordingly, the thesis intends to contribute to enhancing sustainability in urban transport systems through improvement of energy efficiency and reduction of both local and global air pollution.

1.3 Literature review and identified gaps

The topical challenges, as stated previously in Section 1.1, have raised the demand to act. Research focused on many aspects and factors that need to be taken into consideration for finding viable solutions to achieve the climate target and particularly decarbonise the road transport sector. This section is dedicated to summarising the efforts and work done by others, and based on that, to point out identified gaps in the knowledge base and how this doctoral thesis closes those.

This literature review is split into three parts that consecutively built upon each other: 1) literature on energy use, GHG emissions, and costs of hybrid-electric and plug-in hybrid-electric buses; 2) literature on management strategies for the charging schedule and all-electric operation of plug-in hybrid-electric buses; 3) literature on the representation of real-world behaviour and quantifying uncertainties in long-term energy systems modelling.

Accordingly, the knowledge base evolves over the three parts by scaling up the scope of considerations, starting from the direct comparison of bus technologies — the bus technology level; to the management of an electrified bus fleet and necessary charging infrastructure in operation — the bus fleet management level; and finally to the planning and impact assessment of transformations of energy and transport systems — the long-term system planning level.

At the end of each review subsection, identified gaps are pointed out and an associated research question is derived. For a direct overview on all research questions in this thesis, see Section 1.4.

Energy use, GHG emissions and costs of hybrid-electric and plug-in hybrid-electric buses

The first part of this literature review gives an overview on research on the measurement and evaluation of energetic, environmental and economic aspects of different types of buses. Those research findings can support the decision process for selecting particular types of buses that shall be tested and operated in bus transport systems.
A categorisation of buses can be made based on technological features, such as the powertrain, chassis and fuels. The focus in this literature review is on buses having either conventional, hybrid-electric or plug-in hybrid-electric powertrains. As transition technologies are the topic of this thesis, technologies such as battery-electric and fuel cell buses are excluded either due to their issue of range anxiety (Electrification Coalition, 2009) and resulting strong dependency on charging infrastructure for a reliable operation as in the case of battery-electric buses (Mahmoud et al., 2016), or due to the lack of hydrogen infrastructure and its high production cost as in the case of fuel cell buses (Hua et al., 2014). In addition, the chassis is considered, since it is typically specifically designed for certain operation conditions as well as to provide a certain passenger carrying capacity in the bus transport system.

Three types of chassis are considered in this thesis, namely two-axle, articulated and bi-articulated chassis (Figure 2). Those are typically dimensioned as follows: A two-axle bus is built on a single-section chassis having two axles. This chassis has typically a length of around 12 meters and a passenger carrying capacity of 70–90 passengers. An articulated bus is built on a two-section chassis having one pivoting joint and three axles. This chassis has typically a length of around 18 meters and a passenger carrying capacity of 140–170 passengers. Lastly, a bi-articulated bus — or sometimes so-called double-articulated bus — is built on a three-section chassis having two pivoting joints and four axles. This chassis has typically a length of around 25 meters and passenger carrying capacity of 230–250 passengers.

Concerning fuels, a very common fuel for buses is diesel, which is also the typical fuel in case of Curitiba (BRTdata, 2019a). Diesel can be produced either from petroleum crude oil that is referred to as petroleum diesel, or bioresources that is referred to as biodiesel, or a fuel blend consisting of both petroleum diesel and biodiesel that is referred to as biodiesel blend. Although other types of fuels also exist, those are outside the scope of this thesis as the focus is on the evaluation of powertrains and chassis for buses. Notably is that all aforementioned types of powertrains, chassis and fuels are commonly used in the design of buses, such as those operated in the city of Curitiba (URBS, 2019).

The use of the hybrid-electric powertrain technology in two-axle buses has been proven to be an energy saving measure for buses in their operation phase compared to conventional buses. Since the two-axle bus is very commonly used in bus transport system, a considerable amount of research was carried out for this type of bus. Some studies identified fuel savings of 35% in the case of Gothenburg, Sweden (Hellgren, 2007); 23–28% in the case of the US state of Iowa (Hallmark and Sperry, 2012); 19–35% for various different cases and associated driving cycles, i.e. driving cycle refers to the driving pattern of a vehicle represented by data points stating speed versus time or distance (Nylund et al., 2012); 18–29% in the case of Beijing, China (Zhang, Wu, Liu, Huang, Yang, et al., 2014); 30–50% in another case in China (Guo et al., 2015); ~15-50% for standardised driving cycles (Lajunen, 2012b); (6±12)% in the case of Hong Kong (Keramydas et al., 2018); 20% in the case of Brazil (D’agostino and Ribeiro, 2004); and 27–31% in a case in China (Hu et al., 2009). The main reason for the considerable energy savings is the higher energy-efficiency of electric motors in comparison to internal combustion (diesel) engines.

![Figure 2: Illustrations of two-axle, articulated and bi-articulated buses (URBS, 2019)](image-url)
Moreover, the capability of using an on-board regenerative braking system improves the energy efficiency, since excess braking energy is recovered and converted into electricity. This internally generated electricity can be again used in the electric motor then. A regenerative braking system is particularly advantageous for operation in urban driving conditions (Soylu, 2014), where usually a frequent alternation happens between acceleration and braking. To provide an estimation, a regenerative braking system can recover 21–52% of the potential energy loss in the braking process, which is again available for propulsion then (Perrotta et al., 2012; Soylu, 2014).

An observation from the various studies is that their results for energy saving estimations can significantly differ. The reasons are different driving patterns in the respective cases as well as different types of conventional buses and hybrid-electric buses that were compared to each other. This implies different states of technologies, too. One indicator for the state of a deployed technology in a bus is the Euro emission standard. Emissions of a bus decrease with an increasing Euro emission standard according to the requirements set by (European Commission, 2011; European Commission, 2009) as well as this was shown together with the observation of a decreasing energy use trend in the study by (Zhang, Wu, Liu, Huang, Yang, et al., 2014).

While hybrid-electric powertrains have been proven to be an effective measure for energy savings, they do not usually have the possibility to store a large amount of electricity due to rather small on-board batteries in terms of nominal capacity. This leads to a depletion of the battery over time, i.e. the state-of-charge (SOC) decreases. SOC is the analogous to the fuel gauge in a conventional vehicle and states the percentage of available charge to the nominal capacity in the battery. Plug-in hybrid-electric powertrains usually employ larger batteries than hybrid-electric powertrains; start their operation with a charged battery from the bus depot; and are designed for opportunity charging. Overall, the larger amount of usable electricity increases the all-electric range and thus, more distance can be driven with electricity instead of diesel. Concerning the energy saving potential, studies showed a clear energy efficiency increase with increasing degree of electrification, e.g. the study by (Lajunen, 2012b). While hybrid-electric two-axle buses save 15–50% of energy based on the studies cited in the previous paragraph, simulations showed an energy saving potential for plug-in hybrid-electric two-axle buses compared to conventional buses of ~70% for different driving cycles (Lajunen, 2012b); ~44% for a mix of standardised driving cycles incorporating urban, suburban and highway driving patterns (Suh et al., 2012); a powertrain energy efficiency of ~36% — giving ~9 MJ/TWh/km of diesel consumption for a plug-in hybrid electric bus operated in Gothenburg, Sweden (Hu et al., 2013), which amounts to 44% of fuel savings when compared to ~16 MJ/TWh/km of diesel consumption for a conventional bus as found for the same case by (ELECTRICITY, 2016); 50–65% of energy savings for a case study on a bus route in Gothenburg, Sweden (ELECTRICITY, 2016); 5–9% of fuel savings in the case of Wake County, North Carolina, USA (Choi and Frey, 2010); and 30–40% higher energy efficiency for six city bus driving cycles (Gao et al., 2016).

The previous studies showed that findings can vary between different bus technologies as well as between locations due to different driving cycles. Some studies used standardised driving cycles, whereas some other studies used driving cycles derived from recorded real-world driving patterns or actual real-world tests. Real-world driving cycles can strongly differ from standardised driving cycles or dynamometer tests (Wu et al., 2012), especially for urban driving patterns (Ribau et al., 2014; Soylu, 2014). Thus, real-world driving cycles should be used to generate case-specific insights and conclusions.

Another influential factor is the passenger load (Ribau et al., 2015; Q. Yu et al., 2016). It states the aggregated weight of all passengers that are simultaneously transported in a bus. In this
In addition to technological aspects, such as powertrain and chassis, other factors influence the operation and likewise, energy use of buses. Many factors are related to the road network design (Yang et al., 2014). The latter includes and/or influences traffic flow (He et al., 2013), driving cycle (Lajunen, 2014a; Nylund et al., 2012), operation time (Zhang, Wu, Liu, Huang, Yang, et al., 2014) and elevation profile (Lajunen, 2014b).

Moreover, driver behaviour is an operational uncertainty in energy use estimations, i.e. an uncertainty during the operation. Thus, its impact assessment is important to inform about its relevance for certain bus technologies. This has been shown, for example, by the positive effect of eco-driving training on energy savings of buses, e.g. energy savings of 5–7% were achieved in the case of Atlanta, USA (Xu et al., 2017); ~7% in a case study in Sweden (Strömberg and
Karlsson, 2013); 10–15% in the case of Athens, Greece (Zarkadoula et al., 2007); and 17% in the case of Porto, Portugal (Perrotta et al., 2014). Hence, bus driver behaviour can considerably influence the energy use of a bus.

Energy use, GHG emissions, local air pollution and noise are often directly linked to the use of fuels derived from fossil resources. Since the combustion of liquid fuel in an internal combustion engine generates CO₂ emissions, similar magnitudes for reduction potentials of CO₂ emissions in the operation phase can be found as in the aforementioned studies for energy savings. The magnitude is similar due to the linear relationship between combusted fuel and released CO₂. The carbon (C) in a liquid fuel is combusted and reacts with oxygen (O₂) from the air that together form carbon dioxide (CO₂). The amount of non-combusted carbon is negligible and is even suggested to be excluded by the Intergovernmental Panel on Climate Change (IPCC) (IPCC, 2006, p.2; IPCC, 2000). Moreover, the amounts of other GHG emissions, such as methane (CH₄) and nitrous oxide (N₂O), are negligible during the operation phase of road vehicles when compared to the amount of CO₂ emissions (Becker et al., 1999; Nam et al., 2004).

In addition to energy use and GHG emissions, economic aspects must be considered for a successful transformation. Studies have shown that advanced buses can compete with conventional buses also concerning cost. For example, in a case study in Sweden, (Nurjadi et al., 2014) found 7% and 17% lower total cost of ownership for hybrid-electric and plug-in hybrid-electric buses, respectively, when compared to a conventional bus fuelled with petroleum diesel. In the case of Curitiba, the cost of transport service is used to calculate the fare for paying passengers (URBS, 2018b). The largest amount of cost accounts for salaries for the personnel to operate and administrate the bus transport system (URBS, 2018a). The second largest proportion is the fuel cost that account for 17% of the cost of transport service (URBS, 2018a). The fuel cost is influenced by the energy use of a bus as well as the fuel price. In the case of Brazil, fuel prices have been fluctuating over time (ANEEL, 2018; ANP, 2018b) and add another source of economic uncertainty for bus operators.

The first part of this literature review showed that many scientific studies exist on estimating energy use and GHG emissions of conventional, hybrid-electric and plug-in hybrid-electric two-axle buses. However, only a few studies exist for articulated buses and comparisons of different bus technology to each other. Furthermore, no study was found that estimates the energy use of bi-articulated buses. This leads to the following first research question:

1. **How much can energy use, GHG emissions and cost of transport service be reduced by advanced buses?**

This first research question also includes the consideration of some influential factors, such as the analysis of bus routes, operation times, passenger loads, driving cycles and fuel prices on the different types of buses. Moreover, uncertainties are quantified, and scenarios, in which the bus fleet composition is changed, are simulated to evaluate the implications of findings on the cost of transport service as well as service quality. The case study approach is very important for finding answers to the first research question as different types of buses should be analysed and evaluated based on the same traffic conditions, i.e. driving cycles and elevation profiles. Overall, the research question contributes to knowledge creation at the bus technology level.

**Management strategies for the charging schedule and all-electric operation of plug-in hybrid-electric buses**

The second part of this literature gives an overview on research on methods, tools and algorithms to (re)design bus transport systems. The focus is on the introduction and operational
optimisation of electrified bus fleets concerning energy management and operational uncertainties. Those research findings can support the planning phase in a transformation of a bus transport system as well as can optimise the operation of an already introduced electrified bus fleet. Management strategies for electrified bus fleets become particularly important once those include a larger number of plug-in hybrid-electric and/or electric buses, e.g. when many conventional buses are replaced by plug-in hybrid-electric buses.

For the (re)design of bus transport systems, research focused on the general design of electrified bus transport systems considering strategic and operational requirements (Göhlich et al., 2018), including necessary operational changes to introduce plug-in hybrid-electric buses (Häll et al., 2019). Many studies were carried out to plan charging infrastructure considering, e.g. the bus fleet composition (Rogge et al., 2018); the influence of operational uncertainties (Vepsäläinen et al., 2019); charging stations and the power grid connection scheme (Lin, Zhang, Shen and Miao, 2019); and electricity demand (He et al., 2019).

Different charging technologies exist that were analysed, e.g. planning of a facility for battery-swapping (An et al., 2019); techno-economic analysis of charging technologies (Nicolaides et al., 2019); infrastructure planning of wireless chargers for dynamic charging, i.e. charging is done while a bus is driving (Helber et al., 2018); design of wireless charging systems based on reinforcement learning algorithms (Lee et al., 2019); and comparison of charging technologies considering life-cycle cost and charging requirements (Lajunen, 2018). Life-cycle aspects were also considered by (Bi et al., 2018) who analysed the deployment of charging stations based on multi-objective life-cycle optimisation.

The identification of locations for charging stations was in particular subject in many studies, e.g. studies by (He et al., 2018; Liu and Song, 2017; Xylia et al., 2017). Locations and dimensioning of charging stations were analysed by using spatial-temporal models (Lin, Zhang, Shen, Ye, et al., 2019) as well as with the goal to minimise cost while considering also vehicle procurement (Wei et al., 2018). The dimensioning of chargers was assessed in studies to enhance understanding of power requirements (Ranta et al., 2016); or to analyse the trade-off between dimensioning of the on-board battery in a bus versus dimensioning of charging infrastructure (Kunith et al., 2017). The latter should also include the consideration of timetables and routes (Gao et al., 2017; Rogge et al., 2015). Moreover, other trade-offs were identified, such as a trade-off between charge time and number of charging stations (Sebastiani et al., 2016); a trade-off between robustness and cost of a charging system (Liu et al., 2018); and cost-competitiveness of charging infrastructure (Chen et al., 2018).

All the aforementioned studies have provided important insights to start a transition of public bus transport systems towards more electrification by analysing case studies and/or starting proof-of-concept projects.

Regardless whether only one plug-in hybrid-electric bus is operated or a large bus fleet, some management is required to achieve effective opportunity charging without compromising the punctuality of the transport service. Thus, with the inauguration of plug-in hybrid-electric buses comes the necessity to set management strategies for the charging schedule at fast charging stations and preferably, some planning where and when to drive all-electric. To support the planning phase, a few studies focused on the charging schedule of buses. For example, (Niekerk and Akker, 2017) analysed the case that buses are recharged in a bus depot. However, since the bus depot can be potentially far away from the current position of a bus in operation, other studies also considered the case of opportunity charging on bus routes, e.g. (Qin et al., 2016). While the prevention of range anxiety and ensuring reliability of the transport service are crucial
for a successful transition, some studies aimed to minimise operating cost at the same time (Qin et al., 2016; Yang et al., 2018), or to minimise peak loads in the power grid (Jahic et al., 2019).

A common limitation is the assumption of average energy use values rather than the actual route-specific and time-specific energy use as a result of the driving cycles of buses and elevation profiles of the bus routes. The reason is often a lack of real-world bus operation data. Hence, studies often assume an operation of buses according to an idealised timetable schedule of the bus transport system. This, however, can neglect operational uncertainty, such as car accidents, congestion, or any other unexpected interruption, that eventually can result in a deviation from the timetable. Moreover, the energy use of buses can strongly depend on the bus route and operation time (Suzdaleva and Nagy, 2018; Rahman et al., 2018; Tao et al., 2018), and can significantly differ from standardised driving cycles (Millo et al., 2014; Wang et al., 2015; Xu et al., 2015; Yay et al., 2016; Zhang, Wu, Liu, Huang, Un, et al., 2014).

The aim should be to use energy use data based on route-specific and time-specific driving cycle data, i.e. real-world driving cycle data, and elevation profile data in optimisation models. Thus, a more flexible approach is needed that can adjust to potential deviations due to operational uncertainty. In this regard, real-time optimisation (RTO) is a much more flexible approach than the static assumption of an idealised timetable. RTO is a control technique that gives periodic feedbacks to adjust the charging schedule and/or all-electric operation of buses. For example, in periodic time intervals, information about the geographical positions and state-of-charge of buses are collected. This information is then used in an optimisation model. The solution from the optimisation contains the decisions that are sent to the buses, for example, concerning their allocation to charging stations, charge time and all-electric operation. Thus, the periodic adjustments shall react on potential deviations from the timetable to improve the allocations to charging stations and charge times of buses as well as to maximise all-electric operation. A few studies already exist in the literature that presented some analyses considering RTO. (H. Yu et al., 2016) used RTO to optimise the energy management system in an electric bus with the aim to reduce energy use and costs. (Paul and Yamada, 2014) used RTO to maximise the total all-electric distance of a battery-electric bus fleet that was operated on four bus routes in the case of Japan and complemented by conventional buses.

The second part of this literature review showed that many studies provide insights for the planning phase in the transformation of a bus transport systems towards electrification and decarbonisation. However, the integration of energy use data based on route-specific and time-specific driving cycle data and elevation profile data in optimisation models is quite limited. In this regard, RTO provides a possibility to analyse more dynamic data to address operational uncertainty and to use that data in optimisation models. While (Paul and Yamada, 2014) already analysed the case to maximise the total all-electric distance of a battery-electric bus fleet together with conventional buses as complementary options, some other bus technologies and management strategies could be considered and compared. This leads to the following second research question:

2. What potential exists for energy savings and all-electric operation from the operational optimisation of a plug-in hybrid-electric bus fleet?

The research question also includes the development and conceptual testing of a flexible and scalable real-time optimisation model that can use real-world driving cycle and elevation profile data. Considering the already identified knowledge gap for bi-articulated buses from the first part of this literature, this is another opportunity to extend the scientific literature in this regard. The current situation of operating mainly conventional bi-articulated buses in Curitiba is
compared to hypothetical scenarios in which hybrid-electric and plug-in hybrid-electric bi-articulated buses are operated. For the latter, five different management strategies for the charging schedule and all-electric operation are analysed subject to operational uncertainty. Overall, the research question mainly contributes to knowledge creation at the bus fleet management level, but also creates knowledge at the bus technology level in the case of bi-articulated buses.

**Real-world behaviour and uncertainties in long-term energy systems modelling**

The third part of this literature review gives an overview on research on the utilisation of real-world data to advance real-world heterogeneity in energy systems modelling. Those research findings can support the planning phases in long-term transformations of energy and transport systems, including quantifying of uncertainties and assessing their impacts on insights and conclusions. An indispensable tool to assess future scenarios is a long-term energy systems modelling framework. However, the use of heterogenous real-world data in existing frameworks remains a challenge and is therefore reviewed, too.

Cities have been evolving to data generators for the last years. Digitalisation and the concept of the **smart city** have been popularised in this regard. Although multifaceted meanings and various definitions exist (Joglekar and Kulkarni, 2017), a smart city usually implies measurement of real-world behaviour through information and communication technology (ICT), and the use of that data to improve life quality and efficiency (Albino et al., 2015). An example is the concept of **Intelligent Transport System** (ITS) (Sumalee and Ho, 2018) within the concept of **Internet-of-Things** (IoT) (Čolaković and Hadžialić, 2018). In an ITS, vehicles exchange information with an external computer system. For example, vehicle operation data is sent to a database. There, the data is stored and can be retrieved for the purpose of some analysis. Additionally, the computer system can send information back to the vehicles to provide control signals or other information.

Open data movements have started to provide access to stored data and allow its use and distribution globally (European Data Portal, 2019). While open data is often freely accessible, it does not require this, especially when considering the costs for production, storage and publishing of data (European Data Portal, 2019). A free-access example is the open data platform in Curitiba that stores real-world bus operation data (UFPR, 2019). Open data can differ in size and the ubiquitous term of **big data** is often used in this context. However, not all large datasets can be considered as big data. A distinction can be made based on software and hardware requirements for data storage and processing. Big data typically requires a multi-node cluster database for storage and sometimes a computer cluster for processing (Hashem et al., 2015; Taylor, 2017). In comparison, a large dataset, i.e. not a big dataset, usually fits in an ordinary database, and the capabilities of a single computer are enough for processing. Yet, high computational power and specific methods can still be required to process data time-efficiently (Morley and Parker, 2012), e.g. multiprocessing. Multiprocessing refers to the use of multiple processes to process simultaneously several data files in parallel. According to (Zhang et al., 2017), digitalisation and cross-disciplinary collaboration of professionals provide the possibility to fundamentally change the operation and management of cities. Thus, the new opportunities should be taken that arise from open data initiatives.

Two research foci have been identified in the literature concerning final energy use in energy systems that use large datasets containing real-world data, namely residential buildings and urban transport. Regarding urban transport, for example, (Moreno et al., 2015) presented a new traffic management service that predicts congestion and suggests an alternative route. Implications can be energy savings and emissions reduction due to avoidance of stop-and-go
driving (Giakoumis and Zachiotis, 2018). Other studies used real-world vehicle operation data to estimate energy use and emissions. For example, (De Gennaro et al., 2016) monitored the operation of two car fleets with on-board logging devices in the two Italian provinces Modena (52 834 cars) and Firenze (40 459 cars) during May 2011. The data was used to simulate alternative scenarios in which hybrid-electric and battery-electric cars were operated for the assessment of EU transport policies. (Fetene et al., 2017) analysed two years of real-world data collected from 741 battery-electric cars to increase understanding between the influence of driver behaviour, road type and weather conditions on energy use and all-electric range. A couple of studies analysed real-world data from cabs in the case of China. For example, a spatial-temporal distribution of energy use and emissions was analysed by (Kan et al., 2018) who used real-world data from 6658 cabs in Wuhan; (Luo et al., 2017) who used real-world data from 13 675 cabs in Shanghai; and (Cao et al., 2017) who used real-world data from cabs in Guangzhou. (Guo et al., 2017) analysed, in addition to cabs, also buses and the metro system in Shanghai to estimate the benefits of having all three transport modes concerning travel cost and time. Overall, applied research utilising large amounts of real-world data has increased concerning the understanding of energy use and emissions from large operating vehicle fleets. And, for example, the estimations and findings of these studies could be used as input data in the final energy demand side in long-term energy systems models.

Many long-term energy systems modelling frameworks are at their core techno-economic optimisation model, i.e. an optimal solution is searched to a problem that requires the evaluation of technology investment options. An optimisation model typically consists of decision variables, parameters and index sets that are logically linked to each other and limited by constraints in form of equations. The very first equation usually defines the objective function that states the goal of the optimisation model. Eventually, a solver maximises or minimises the objective function considering all constraints.

Three design types of optimisation models are distinguishable: Deterministic models having fixed input values for parameters; stochastic models having random input values for parameters; and hybrid models having a mix of both fixed and random values for parameters. Concerning the output data from a model, i.e. the optimal solution, deterministic models always produce the same output data from the same input data, whereas stochastic and hybrid models most likely produce different output data due to the variability of random values for parameters.

The modelling process — from the development of a modelling framework by developer(s), to its application by user(s), and eventually to generated insights and conclusions that are read and potentially used by reader(s) of a study — is shown together with uncertainties and uncertainty analysis methods in Figure 3.

Uncertainty is a ubiquitous topic in systems modelling and analysis that can be generally defined as: “… any deviation from the unachievable ideal of completely deterministic knowledge of the relevant system.” (Walker et al., 2003). The assessment of uncertainty is therefore crucial to understand the reliability of insights and conclusions (JCGM, 2008). Uncertainty can be induced during the design process of a modelling framework — referred to as endogenous uncertainty in this thesis (Figure 3). For example, the developer of a modelling framework makes assumptions on the objective function and relationships between decision variables and parameters through the definition of constraints. Additionally, uncertainty can be induced by the user during the application of a modelling framework through the input dataset — referred to as exogenous uncertainty in this thesis (Figure 3). The user might subconsciously induce exogenous uncertainty during the data compilation and creation of the input dataset. For example, a
difference could exist between the true value, i.e. the value in the real world, and the measured value, i.e. the value used in the dataset. Potential reasons are inaccurate measurement devices and/or imprecise measurement practices (JCGM, 2008). Moreover, other error sources could be a mistakenly use of values for the dataset due to ambiguity in the use or interpretation of data (Grünbaum, 2007) as well as imperfect definitions in data sources (Belussi et al., 2007). Additionally, lack of data can lead to the necessity to make assumptions. Thus, informing the reader of a study about potential impacts on insights and conclusions is therefore of high importance.

The compilation of the dataset is not simply done by collecting data and putting that into a structured format. Certain data is sometimes unavailable. In that case, assumptions and judgements by researchers and analysts are required that, however, also induce exogenous uncertainty into the dataset (Spiegelhalter and Riesch, 2011). Presupposing the adherence of scientific measurement practices and unambiguous definitions in the creation of a dataset, that dataset shall be considered as is for its application in a modelling framework then. Nevertheless, the input dataset is an underlying assumption in the modelling process and ultimately, induced uncertainty is passed on to insights and conclusions obtained from a model.

Various uncertainty analysis methods exist to assess both endogenous and exogenous uncertainty and to inform the reader of a study, e.g. by providing a list of possible outcomes, stating a probability distribution for an outcome, or qualitative statements that uncertainty exists and may have a positive or negative effect on an outcome, etc. (Spiegelhalter and Riesch, 2011).

![Figure 3: Modelling process, uncertainties and uncertainty analysis methods](image-url)
Endogenous uncertainty can be assessed by disclosing the source code of the modelling framework, i.e. through open source code. Thus, both the user of the modelling framework and reader of the study can review logic and assumptions implemented by the developer, and potentially assess logical and numerical influences on the output data, insights and conclusions. In addition to open source code, an open dataset can enhance transparency and enables the reader to assess exogenous uncertainty, such as a review of assumptions. Another common method is scenario analysis to assess endogenous uncertainty. This method is often applied in form of narratives to assess the influence of different sets of input data on insights and conclusions. A deeper understanding of the influence of parameters on the output data can be obtained by using sensitivity analysis. Since a sensitivity analysis can be quite work intensive, this uncertainty analysis method is often limited to only a few key parameters. However, as (Weijermars et al., 2012) suggest, an extensive sensitivity analysis together with an unambiguous explanation of the underlying methodology would be desired for a comprehensive understanding of uncertainty. Last but not least in this list of uncertainty analysis methods, a Monte Carlo simulation can be used to assess the influence of stochastic behaviour of input data on insights and conclusions. This method uses random sampling of input values for parameters to estimate the probability of certain insights and conclusions. The importance of a Monte Carlo simulation is further elaborated considering real-world data and common assumptions in the following.

Variations of physical quantities and their real-world values can lead to an incomplete picture of findings, e.g. if only one value, such as an aggregated average value, is used as input data rather than the possible probability distribution of values around the average value. Considering again the aforementioned studies, the study by (Fetene et al., 2017) provides a probability distribution of energy use data for the case of cars. Thus, this distribution could be used to represent more of the real-world heterogeneity in an energy systems model. This can be done by a Monte Carlo simulation that enables an estimation of the associated exogenous uncertainty and its impact on insights and conclusions. Nevertheless, in addition to probability distribution data, a long-term energy systems modelling framework is needed that can handle such probability distribution data — preferably as open source tool for transparency of research findings. However, not only open data, but also open source code is a backlog demand in applied research fields according to (Pfenninger et al., 2017). No exception is the field of energy systems research considering the review paper by (Hall and Buckley, 2016). The study identified only a few models out of 96 models and simulation tools that are open source in the case of the UK. Reasons could be a deficiency of development guidelines for real-world energy systems and varying data quality of heterogeneous data according to (Pfenninger et al., 2017). Besides, only a few academic open source modelling frameworks exist, such as Balmoral (Wiese et al., 2018), Temoa (Hunter et al., 2013) and OSeMOSYS (Open Source energy MOdelling SYstem) (Gardumi et al., 2018; Howells et al., 2011). Out of these three models, (Groissböck, 2019) concludes that only Temoa and OSeMOSYS are advanced enough for serious use based on an evaluation of the functionality.

Temoa offers the possibility to perform stochastic optimisation, whereas OSeMOSYS does not offer this in any of its code implementation, i.e. neither in the code version written in GNU MathProg (GNU MathProg, 2015), GAMS (GAMS Software GmbH, 2019) nor Python-Pyomo (Hart et al., 2017; Hart et al., 2011). The OSeMOSYS modelling framework has been widely used by the scientific community, e.g. in studies by (Anjo et al., 2018; Brozynski and Leibowicz, 2018; Burandt et al., 2019; Chung et al., 2019; de Moura et al., 2018; Dhakouani et al., 2017; Groissböck and Pickl, 2018; Keller et al., 2018; Leibowicz, 2018; Leibowicz et al., 2018; Lößfler et al., 2017; Niet et al., 2018; Palmer-Wilson et al., 2019; Peña Balderrama et al., 2018; Pinto de Moura et
al., 2017; Riva et al., 2019; Moksnes et al., 2017; Welsch et al., 2014). Furthermore, OSeMOSYS is used as a teaching tool (OpTIMUS, 2019). However, OSeMOSYS is deterministically designed, i.e. a model instance always produces the same output dataset to the same input dataset. Consequently, the associated uncertainty of a model parameter and value from the input dataset are not accounted. Yet, (Martiauskas et al., 2018) and (Leibowicz, 2018) could run stochastic simulations with OSeMOSYS, but relied on additional tools. The combination of tools is quite inconvenient though. While (Leibowicz, 2018) developed a stochastic version of OSeMOSYS in GAMS, it needs to be noted that the algebraic modelling language GAMS is not fully open source. The combination of tools is quite inconvenient though. While (Leibowicz, 2018) developed a stochastic version of OSeMOSYS in GAMS, it needs to be noted that the algebraic modelling language GAMS is not fully open source. A link between Temoa and OSeMOSYS is not a viable solution either, because of their different designs. Moreover, the extension of an existing model is more promising than linking different models according to (Timmerman et al., 2014).

The third part of this literature review showed that real-world datasets and open data have gained in scientific importance (Pfenninger et al., 2017). Their utilisation in long-term energy systems modelling remains a challenge though, since the use of real-world dataset and capturing of the associated real-world heterogeneity requires new functionalities. Open data and open source tools are still backlogs in applied research field and also in the specific area of energy systems modelling (Pfenninger et al., 2017). This leads to the following third research question:

3. How can the influence of real-world uncertainty be represented in and quantified with the long-term energy system modelling framework OSeMOSYS?

This research question includes the development of a Monte Carlo simulation feature for the long-term energy systems modelling framework OSeMOSYS, which is implemented in a new code implementation named OSeMOSYS-PuLP. OSeMOSYS-PuLP is a software system that extends the capabilities of the OSeMOSYS modelling framework by a Monte Carlo simulation in an automated and convenient way. Overall, a methodological framework for an empirical deterministic-stochastic modelling approach to utilise real-world datasets in long-term energy systems modelling is presented including a proof-of-concept case study for OSeMOSYS-PuLP using the open bus operation data from Curitiba. The new tool can be used to quantify the impact of exogenous uncertainties on insights and conclusions from an energy systems model. Overall, the research question contributes to knowledge creation at the long-term system planning level.
1.4 RESEARCH QUESTIONS, SCOPE AND RELEVANCE

Research questions

Three research questions, as previously derived from the literature review, are answered in this doctoral thesis:

1. How much can energy use, GHG emissions and cost of transport service be reduced by advanced buses?

2. What potential exists for energy savings and all-electric operation from the operational optimisation of a plug-in hybrid-electric bus fleet?

3. How can the influence of real-world uncertainty be represented in and quantified with the long-term energy system modelling framework OSeMOSYS?

Scope

This thesis focuses on the transition phase of bus transport systems from operating conventional buses to using electrified buses by exploring electrification as a vector for decarbonisation. The term transition technologies concerns the transition phase and refers to technologies that can use or support the use of electricity in bus transport systems for passenger transport without relying exclusively on electricity as an energy source for operation. For example, hybrid-electric and plug-in hybrid-electric buses have both an electric motor and an internal combustion engine for propulsion and can be considered as transition technologies that are technologically situated between conventional buses (only an internal combustion engine for propulsion) and battery-electric buses (only an electric motor for propulsion). Additionally, tools and models are considered that can support and optimise the transition phase. In summary, this leads altogether to the thesis’ title Transition Technologies for Electrification and Optimisation of Bus Transport Systems. The C40-city of Curitiba in Southern Brazil is used as a case study.

Different bus technologies for the transition phase are analysed and evaluated regarding energy use, GHG emissions and cost of transport service. The main focus is on the operation phase of buses and the potential opportunities when replacing conventional technologies as well as optimising the operational management of a plug-in hybrid-electric bus fleet subject to operational uncertainty. Moreover, the research developed a new open source tool OSeMOSYS-PuLP for adding the feature of a Monte Carlo simulation to the long-term energy systems modelling framework OSeMOSYS. Notably is that the application of this tool is not limited to the planning of bus transport systems and can be applied in research addressing a broader scope concerning the transformation of transport and energy systems.

The findings state advantages and disadvantages of different bus technologies; available potentials for energy savings and all-electric operations of plug-in hybrid-electric buses; and a methodological framework to capture and account more real-world heterogeneity in long-term systems modelling based on open data and open source tools. The latter can be particularly relevant for research addressing the planning phase of a system’s transformation, in which decision-makers are supported with information about opportunities and impacts coming along a transformation.

The target audience of this thesis are researchers, analysts and decision-makers in the area of transport and energy systems planning.
Relevance
In the city of Curitiba, the operating bus fleet consists of 1229 buses of which 30 buses employ hybrid-electric powertrains at present (URBS, 2019). The 30 buses are a first effort to introduce more technological advanced buses, that can use electricity to drive, in the city with the goal to reduce both energy use and emissions. Additionally, some real-world proof-of-concept projects were carried out to test other types of advanced buses within real-world operation conditions during the period 2015–2017. Those include the operation of 1) a hybrid-electric articulated bus (Volvo Bus Corporation, 2017), 2) a plug-in hybrid-electric two-axle bus (Volvo Bus Corporation, 2017) and 3) a battery-electric two-axle bus (URBS, 2015a). One fast charging station was implemented during the test period to enable opportunity charging for the plug-in hybrid-electric bus. The battery-electric bus was charged through slow charging at a depot overnight (URBS, 2015a).

Obviously, Curitiba has tested a mix of different bus and charging technologies. Yet, the city is still at the beginning of transforming its public bus transport system towards the operation of a large electrified bus fleet. Note: Real-world tests 1) and 2) were carried out in the scope of the research project Smart City Concepts in Curitiba in which also the research work of Paper I, Paper II and partly Paper III was done. Consequently, insights generated from the three studies also complement knowledge gained from the real-world tests 1) and 2).

The development and test scope in Curitiba are similar to situations in many other cities, i.e. cities in which a few plug-in hybrid-electric or battery-electric buses are operated and charged through opportunity charging at one or a few fast charging stations. Thus, the case of Curitiba can be considered as representative for many other cities that have started a transition phase or plan to do so. For example, first demonstration projects can be found in several cities in Europe (ZeEUS project, 2016), South America (Brittlebank, 2015; Dzikiy, 2019b; UN Environment Programme, 2018), North America (Dzikiy, 2019a; Sustainable Bus, 2019), Asia (Global Mass Transit, 2018), Oceania (Cotter, 2019; EECA, 2019) and Africa (Focus on Transport, 2018; Weston, 2018). Based on these observations, it can be concluded that the electrification of public bus transport systems has started globally. Notably is that a few large-scale implementations already exist, too — especially in the market’s sales leader China (IEA, 2019).

Furthermore, the commitment made by Curitiba as part of the C40 network, i.e. signing the C40 Cities Clean Bus Declaration of Intent (C40, 2015b), is an extra effort within the urban transport sector to contribute to the climate target. Moreover, other networks, commitments and targets outside of the C40 network exist with the goal to change urban mobility and particularly public bus transport systems to reduce energy use and emissions. To name a few here, those include: the provisional agreement to set CO₂ emissions standards for heavy-duty vehicles in the EU that was made by the EU Parliament and the Council in 2019 (European Commission, 2018); the EU network EU Covenant of Mayors for Climate & Energy (Covenant of Mayors, 2019), in which cities make commitments to implement EU climate and energy objectives since 2008; the European Clean Bus deployment Initiative (European Commission, 2017b), that started in 2016; or the Public Transport Declaration on Climate Leadership by the International Association of Public Transport (UITP, 2014), which is an officially recognised collaborative action under the Marrakech Partnership for Global Climate Action (UN Climate Change, 2016), that was launched at the COP 22 in 2016. All these networks — in which commitments are made and/or target are set — are global efforts to reduce energy use and GHG emissions in the road transport sector and particularly from heavy-duty vehicles, such as buses. Decision-makers in cities, public transport authorities and bus operators can often actively choose what type of bus to purchase
and operate. Thus, it is often within their action scope to influence whether to replace an (old) conventional bus by an environmental-friendlier alternative, or not.

The on-going digitalisation of the world and in cities generates new data that enables more advanced management strategies and analyses, e.g. the application of real-time optimisation models to optimise the operation of an electrified bus fleet. Moreover, long-term energy systems modelling frameworks are important tools to test and measure the impact of potential transformations on the environment, society and economy of cities and countries. The development of the new software system OSeMOSYS-PuLP hereby enables the quantification of exogenous uncertainty and can assess its impact and likelihood for insights and conclusions. Notably is that all this insight generation is possible based on open source code with OSeMOSYS-PuLP, which was highlighted by (Pfenninger et al., 2017) as a backlog demand in applied research fields.

In summary, the research questions and scope of this thesis are very topical to Curitiba as well as other cities situated at the beginning or within the transition process of electrifying their public bus transport systems. Hence, the outcomes of this thesis are not only relevant to Curitiba, but the case-specific insights are potentially also transferable and applicable in many other cities globally. Considering international climate agreements, global networks and the commitments by countries and cities, this thesis can support those intentions by providing new analytical advances, new methodological advances, and new data and insights from a different scope of applied research. These advances generate altogether new insights to support data-driven decision-making in the transition phase of bus transport systems from operating conventional buses to using electrified buses.

1.5 OUTLINE OF THE THESIS

This doctoral thesis is written as a compilation thesis (kappa) that summarises and merges the research findings of four scientific papers (Papers I–IV). The consolidated contributions of the papers give answers to the research questions asked in this thesis with the goal to contribute to its stated overarching objective “to support and quantify opportunities in the transition phase of bus transport systems from operating conventional buses to using electrified buses by exploring electrification as a vector for decarbonisation.” (thesis’ objective from Section 1.2). An illustration of the outline of this thesis is shown in Figure 4, including the thesis’ objective, research questions (RQs), levels of consideration (bus technology level, bus fleet management level, long-term system planning level), methods and methodological links between the different modelling types and outcomes.

Chapter 2 — Paper I — compares different types of buses concerning energy use and GHG emissions taking into consideration the operation phase of the buses as well as fuel production and supply. Curitiba’s BRT system is used as a case study. In the same chapter — Paper II —, the cost of transport service is estimated for the buses. The implications are highlighted in scenarios in which the current operating bus fleet is partly or completely replaced by other types of buses. The evaluation considers potential changes of cost of transport service and service quality. Overall, this chapter addresses the first research question and contributes to knowledge creation at the bus technology level.

Thematic link between Chapter 2 and Chapter 3: Once one or more bus technologies are identified from such direct comparisons, a potential (large-scale) replacement and introduction of many advanced buses should be assessed. This also includes the estimation and evaluation of...
potential opportunities that can arise when considering an electrified bus fleet as a system and its operational optimisation.

Chapter 3 — Paper III — compares scenarios in which conventional, hybrid-electric or plug-in hybrid-electric bi-articulated buses are operated. A subsystem of Curitiba’s BRT system is used as a case study. Plug-in hybrid-electric buses need to be recharged during operation to increase the utilisation of their all-electric drive capability compared to conventional buses. Hence, charging infrastructure must be deployed and the operating bus fleet must be managed to allocate buses to charging stations without compromising punctuality of the transport service. The planning and optimisation of an electrified bus fleet in operation is subject to operational uncertainty. This includes interruptions that can occur due to congestion, accidents or other unexpected events during operation in comparison to an ideal timetable. For this type of evaluation, a real-time optimisation model was developed and tested to simulate different management strategies. While first come, first served is one option to allocate buses to charging stations, other management strategies are simulated and evaluated with the aim to maximise energy savings and/or all-electric operation while considering operational uncertainty. Overall, Chapter 3 evaluates optimisation potentials to manage electrified bus fleets once charging infrastructure would have been deployed and structural changes would have happened. Overall, this chapter addresses the second research question and mainly contributes to knowledge creation at the bus fleet management level, and to some extent at the bus technology level in the case of bi-articulated buses.

Thematic link between Chapter 3 and Chapter 4: The planning and optimisation of an electrified bus fleet using charging infrastructure for opportunity charging is subject to operational uncertainty concerning its charging schedule and all-electric operation. This uncertainty leads to a distribution of possible energy use values of the bus fleet during operation. Eventually, this uncertainty and the randomness of the real world can be described by empirical probability distributions. Those, in turn, could be used in long-term energy systems models to develop strategies that include the consideration of operational uncertainty. While long-term energy system modelling frameworks exist, the possibility to consider uncertainty and, for example, to run a Monte Carlo simulation in an automated and convenient way is rather limited.

Chapter 4 — Paper IV — presents a methodological framework to consider real-world heterogeneity and associated uncertainties in long-term energy systems modelling. For this purpose, a new software system was developed that enables to perform a Monte Carlo simulation using the OSeMOSYS modelling framework in a convenient and automated way — OSeMOSYS-PuLP. The Monte Carlo simulation capability of OSeMOSYS-PuLP can be useful as current open data movements give access to large amounts of real-world data. The software system was built exclusively upon open source tools — from the modelling framework, to the programming language, to the solver of the optimisation model. A proof-of-concept case study is presented that uses open real-world bus operation data. The whole public bus transport system in Curitiba is used as a case study. Overall, this chapter contributes to the discourse of using (open) real-world datasets in long-term systems modelling and evaluating the impact of exogenous uncertainties on insights and conclusions from a model. Overall, this chapter addresses the third research question and contributes to knowledge creation at the long-term system planning level.

Chapter 5 states the key messages from the research. The overall contribution and specific contributions to the scientific literature are summarised. Moreover, limitations are described, and based on this, recommendations are given for future work. The thesis finishes off with highlighting the impact that has been achieved so far and its potential value in the future.
**Objective:**
The overarching objective of this doctoral thesis is to support and quantify opportunities in the transition phase of bus transport systems from operating conventional buses to using electrified buses by exploring electrification as a vector for decarbonisation.

**RQs**

1. How much can energy use, GHG emissions and cost of transport service be reduced by advanced buses?
2. What potential exists for energy savings and all-electric operation from the operational optimisation of a plug-in hybrid-electric bus fleet?
3. How can the influence of real-world uncertainty be represented in and quantified with the long-term energy system modelling framework OSeMOSYS?

**Chapter**

- Chapter 2 (Papers I & II)
- Chapter 3 (Paper III)
- Chapter 4 (Paper IV)

**Scopes**

- BRT system, short-term vehicle simulations, fuel pathways, samples from one day of operation data
- Subsystem of BRT system, mid-term bus fleet simulation, two weeks of operation data
- Bus transport system, long-term system model, 1.5 years of operation data

**Methods**

- Two case studies, GREET, ADVISOR (Deterministic models)
- Case study, RTO simulation, Backwards-calculating energy use rate method (Deterministic models)
- Case study, OSeMOSYS-PuLP, Energy use prediction model (Deterministic-stochastic model)

**Outcomes:**
Insights and tools to support and inform analysts and decision-makers in the area of transport and energy systems planning in their decision-making process to develop and assess different technological options and strategies at different levels while considering associated uncertainties. (Chapter 5)

*Figure 4: Outline of the thesis*


2 ENERGY USE, GHG EMISSIONS AND COST OF TRANSPORT SERVICE OF BUSES

This second chapter compares energy use, greenhouse gas emissions and cost of transport service for different types of buses. The buses are evaluated for selected BRT routes and operation times in Curitiba. Based on the findings, potential implications are presented in scenarios. Those are evaluated concerning cost of transport service and service quality. The research presented in this chapter is based on scientific papers I and II (referenced as Paper I and Paper II).

2.1 ENERGY USE AND GREENHOUSE GAS EMISSIONS

The service of road transport requires considerable amounts of energy to move vehicles carrying passengers and/or goods. Furthermore, energy use and anthropogenic GHG emissions are strongly linked due to the predominate consumption of fossil fuels in this sector. Moreover, combustion engines are mainly employed that emit, in addition to gaseous and particulate emissions, also noise.

At the time of the research presented in Paper I and Paper II, a biodiesel blending mandate was already taken into effect in Brazil. The mandate required that 7% biodiesel was blended into petroleum diesel. This fuel is referred to as biodiesel blend B7 and was considered as reference fuel in the following analyses. The main feedstock for biodiesel are soybeans in Brazil (ANP, 2018a). While the proportion of biodiesel produced from soybeans substituting petroleum diesel can avoid similar percentage of non-biogenic GHG emissions in the operation phase (Nylund et al., 2012), more or less the same amount of energy content is needed in an internal combustion engine when using a biodiesel blend compared to petroleum diesel (Lapuerta et al., 2008). Consequently, the blending mandate does neither reduce a mentionable amount of energy use nor noise. Therefore, alternative powertrain technologies in buses are needed to reduce both energy use and emissions. However, the introduction of those technologies requires major investments for a city and bus operators. Hence, new advanced technologies in buses should be evaluated before purchases are made.

In Paper I, buses were assessed based on a Well-to-Wheel (WTW) analysis as shown in the methodological framework in Figure 5. The WTW scope includes the fuel cycle that consists of two parts: 1) fuel production and supply, also referred to as Well-to-Tank (WTT) scope; and 2) fuel use in buses, also referred to as operation phase or Tank-to-Wheel (TTW) scope, i.e. a TTW analysis accounts the energy flow in a bus from the fuel in the fuel tank — or electricity from the battery — to the rotation of the wheels.

The WTW scope is a common evaluation scope for road vehicles in general and for buses, e.g. applied in studies by (Correa et al., 2017; Nurhadi et al., 2014; Silva et al., 2006). Besides, the WTW scope is an accepted scientific reference by the European Commission to evaluate jointly fuel pathways and vehicles (European Commission, 2016a), i.e. evaluations are possible at the bus technology level. While the focus of this thesis is mainly on the operation phase of buses, it also considers fuel production and supply. This provides estimations for avoided WTT energy expended and WTT emissions released during fuel production and supply as a result from energy
efficiency improvements in the operation phase. Thus, estimations were made based on the common WTW scope.

The distinct difference between a WTW analysis and a life cycle assessment (LCA) is the exclusion of production and disposal of both vehicles and facilities (European Commission, 2016a). While this exclusion is a limitation in a WTW analysis, the WTW scope still provides a meaningful indication as it accounts for most of the life-cycle energy and GHG emissions in the case of buses. For example, the WTW scope of a conventional bus accounts for 90% of its life-cycle energy and GHG emissions (García Sánchez et al., 2012). In case of a more advanced bus, the WTT scope is more important than the TTW scope due to less TTW energy use during its operation phase (Nordelöf et al., 2014). Besides, additional components, such as an on-board battery, require more materials and manufacturing processes. The study by (Chan et al., 2013) found that the vehicle cycle, i.e. bus assembly and transport as well as the use of materials to build the bus, cause 33.8 gCO₂e/km of GHG emissions, measured in grams of carbon dioxide equivalent (CO₂e), for a conventional bus fuelled with petroleum diesel. In comparison, the study estimated 45.1 gCO₂e/km for a hybrid-electric bus (Chan et al., 2013). Although the comparison of both numbers provides a considerable relative increase in GHG emissions for the hybrid-electric bus, the vehicle cycle still contributes little when compared to the WTT scope (conventional diesel bus: 364.7 gCO₂e/km; hybrid-electric bus: 214.4 gCO₂e/km) and particularly, the TTW scope (conventional diesel bus: 2030–2090 gCO₂e/km; hybrid-electric bus: 1150–1170 gCO₂e/km). In summary, it can be stated that the WTW scope also accounts for the largest proportion of life-cycle energy and GHG emissions for an advanced bus and thus, this scope can be used to make meaningful statements concerning the climate impact of both conventional and advanced buses. Besides, it can be argued that the production, disposal and recycling phases of a vehicle’s life-cycle depend more on actions by the vehicle manufacturers as well as those impacts are difficult or potentially impossible to be directly influenced by decision-makers in cities, public transport authorities and bus operators. Hence, those life-cycle stages are outside of the scope in this thesis.

**Figure 5: Methodological framework of the WTW analysis (modified figure from Paper I)**
In Paper I, both WTW fossil energy use and WTW GHG emissions were estimated. The GHG emissions estimations were done for non-biogenic GHG and include CO₂, methane (CH₄) and nitrous oxide (N₂O). Their combined 100-year global warming potential including climate-carbon cycle feedbacks is presented in the unit CO₂e using conversion factors of 1, 34 and 298 for CO₂, CH₄ and N₂O, respectively (Myhre et al., 2013).

The GREET (Greenhouse gases, Regulated Emissions, and Energy use in Transportation) model (ANL, 2016) was used to create fuel pathway models for the production and supply of petroleum diesel and biodiesel produced from crude oil and soybeans, respectively, i.e. analysis of the WTT scope. The WTT analysis estimated the amounts of WTT fossil energy and WTT GHG emissions that were expended or released, respectively, for the provision of one energy unit (megajoule, MJₜₚ₅) of liquid fuel to the buses. The factors for WTT fossil energy use and WTT GHG emissions for biodiesel blend B7 were calculated based on the volumetric shares of its components, i.e. WTT fossil energy use and WTT GHG emissions from 93% of the fuel pathway for petroleum diesel and 7% from the fuel pathway for biodiesel. Additionally, the values of the two factors were estimated for electricity generated from the Brazilian electricity mix consisting of 75.18% hydropower, 8.46% natural gas, 6.38% biomass, 3.55% oil, 2.90% nuclear, 2.56% coal and 0.97% other energy sources (ANL, 2016).

The TTW fossil energy use was estimated considering the carbon content in the fuel, i.e. 93% in the case of the biodiesel blend B7. The TTW GHG emissions were estimated using a carbon balance method. This method presumes that all carbon in the fuel is combusted and is eventually converted into CO₂ in the atmosphere. Other GHG emissions from the combustion process were neglected in the TTW analysis, such as methane (Nam et al., 2004) and nitrous oxide (Becker et al., 1999), due to their marginal contribution compared to the emitted CO₂ during operation. A summary of the WTT, TTW and WTW factors for fossil energy and GHG emissions is provided in Table 1.

Next, the TTW energy use of the buses was estimated and related to driving of one kilometre (km) and one passenger-kilometre (pkm). The functional unit pkm states the aggregated number of passengers travelling together in a transit vehicle, e.g. 20 passengers travelling one kilometre together amounts to 20 pkm.

<table>
<thead>
<tr>
<th>Scope</th>
<th>Estimate</th>
<th>Unit</th>
<th>Petroleum diesel</th>
<th>Biodiesel blend B7</th>
<th>Biodiesel B100</th>
<th>Electricity</th>
</tr>
</thead>
<tbody>
<tr>
<td>WTT</td>
<td>Fossil energy expended</td>
<td>MJₜₚ₅,WTT/MJₜₚ₅</td>
<td>0.180</td>
<td>0.185</td>
<td>0.248</td>
<td>0.485</td>
</tr>
<tr>
<td>GHG emissions expended</td>
<td>gCO₂,WTT/MJₜₚ₅</td>
<td>17.62</td>
<td>18.07</td>
<td>24.05</td>
<td>54.54</td>
<td></td>
</tr>
<tr>
<td>TTW</td>
<td>Fossil energy content</td>
<td>MJₜₚ₅,TTW/MJₜₚ₅</td>
<td>1.00</td>
<td>0.930</td>
<td>0.00</td>
<td>0.00</td>
</tr>
<tr>
<td>CO₂ emissions</td>
<td>gCO₂,TTW/MJₜₚ₅</td>
<td>75.33</td>
<td>70.10</td>
<td>0.00</td>
<td>0.00</td>
<td></td>
</tr>
<tr>
<td>WTW</td>
<td>Fossil energy use</td>
<td>MJₜₚ₅,WTW/MJₜₚ₅</td>
<td>1.180</td>
<td>1.115</td>
<td>0.248</td>
<td>0.485</td>
</tr>
<tr>
<td>GHG emissions</td>
<td>gCO₂,WTW/MJₜₚ₅</td>
<td>92.95</td>
<td>88.17</td>
<td>24.05</td>
<td>54.54</td>
<td></td>
</tr>
</tbody>
</table>
The TTW energy use estimations were obtained using the vehicle simulation tool Advanced Vehicle Simulator (ADVISOR) (Markel et al., 2002; Wipke et al., 1999). ADVISOR was developed by the National Renewable Energy Laboratory (NREL) in the USA with the goal to support vehicle analysis research concerning the development of advanced vehicles (Wipke and Cuddy, 1996). ADVISOR is an open source tool that runs in the MATLAB/Simulink environment (The MathWorks Inc., 2015). Its open source code enables to review the functional principle of a simulation process, including predefined vehicle models and underlying assumptions. Predefined vehicle models can be easily adjusted by inserting case-specific data either through the graphical user interface or directly in the source code. ADVISOR uses the inserted data and scales components accordingly. This provides a high degree of flexibility concerning ADVISOR’s application scope.

During the development of ADVISOR, vehicle models and powertrain component models were validated by academic teams, e.g. through building and testing of hybrid-electric vehicles (Wipke and Cuddy, 1996). Additionally, tests were carried out with proprietary vehicles in the automotive industry. The tests showed a deviation of 2% for estimations in ADVISOR from the real-world tests at that time (Wipke and Cuddy, 1996). The 2%-deviation is attributable to algorithms in ADVISOR that potentially simplify certain physical phenomena, i.e. endogenous uncertainty exists. Nevertheless, the developers of ADVISOR state that the primary source of uncertainty comes from the input dataset (Wipke and Cuddy, 1996), e.g. lack of data resulting in the necessity to make assumptions. While those validation tests were performed rather long time ago, some more recent studies also investigated the accuracy of ADVISOR for various newer and different vehicles. For example, studies by (Ma et al., 2011; Ma et al., 2012) estimated a deviation range of 3–8%. Overall, ADVISOR’s open source design, flexibility and accuracy are reasons for its frequent use in many scientific studies. For example, a wide range of different buses were simulated, such as conventional, hybrid-electric, plug-in hybrid-electric, battery-electric and fuel cell buses — a collectively summarised list for types of bus that were analysed in studies by (Chen et al., 2014; Correa et al., 2017; Lajunen, 2014a; Lajunen, 2012a; Melo et al., 2014; Mirmohammadi and Rashtbarzadeh, 2014; Ribau et al., 2014; Suh et al., 2011; Wang et al., 2017; Yin et al., 2014; Lajunen, 2012b; Khanipour et al., 2007).

<table>
<thead>
<tr>
<th>Powertrain</th>
<th>Chassis</th>
<th>Operation status</th>
<th>PCC</th>
<th>Fuel</th>
<th>Acronym</th>
<th>Paper I</th>
<th>Paper II</th>
</tr>
</thead>
<tbody>
<tr>
<td>Conventional</td>
<td>Two-axle</td>
<td>Yes</td>
<td>85</td>
<td>B7</td>
<td>ConvTwO</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Conventional</td>
<td>Bi-articulated</td>
<td>Yes, Yes</td>
<td>250</td>
<td>B7</td>
<td>ConvBiO</td>
<td></td>
<td>ConvBi</td>
</tr>
<tr>
<td>Hybrid-electric</td>
<td>Two-axle</td>
<td>Yes</td>
<td>79</td>
<td>B7</td>
<td>HybTwO</td>
<td></td>
<td>HybTw</td>
</tr>
<tr>
<td>Hybrid-electric</td>
<td>Two-axle</td>
<td>No</td>
<td>95</td>
<td>B7</td>
<td>HybTwA</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Hybrid-electric</td>
<td>Articulated</td>
<td>Test phase (2016)</td>
<td>154</td>
<td>B7</td>
<td>HybArA</td>
<td></td>
<td>HybAr</td>
</tr>
<tr>
<td>Plug-in hybrid-electric</td>
<td>Two-axle</td>
<td>Test phase (2016)</td>
<td>95</td>
<td>B7, ELC</td>
<td>PlugTwA (PCC: 95)</td>
<td></td>
<td>PlugTw (PCC: 96)</td>
</tr>
</tbody>
</table>
In Paper I, the operation of six different types of buses was simulated on BRT routes in Curitiba (Table 2). The buses are distinguished by their type of powertrain, chassis and operation status in the following. Acronyms are used and compound by type of powertrain (Conv: Conventional; Hyb: Hybrid-electric; Plug: Plug-in hybrid-electric), type of chassis (Tw: Two-axle; Ar: Articulated; Bi: Bi-articulated) and operation status during the period 2015–2017 (O: Operating in Curitiba; A: Alternative — either in a test phase or not operated in Curitiba, yet). Detailed input data for the vehicle models of the buses is provided in Paper I and Paper II.

The BRT system is part of the public bus transport system in Curitiba and spreads radially from the city centre in five directions. BRT routes are designed as high-capacity transport corridors on which mainly conventional bi-articulated buses (ConvBiO) are operated. The remaining five buses in the analysis are either in regular service, in a test phase or could be potential alternatives for Curitiba’s bus transport system (Table 2).

Real-world bus operation data was used to represent real-world driving patterns in the simulations. This data was collected through telematic system from buses that operated on the BRT routes. The dataset contained operation data from seven BRT routes and six operation times during one business day, i.e. samples from one operation day containing a total of 42 driving cycles. Different BRT routes (Table 3) and operation times (morning, forenoon, noon, afternoon, evening and night) were considered to account for potential variation in operation of the buses due to varying traffic conditions on the BRT routes (Kean et al., 2003) and operation times (Zhang, Wu, Liu, Huang, Yang, et al., 2014). BRT routes I and II are declared as express BRT routes in Curitiba, because they have fewer bus stations per kilometre. For example, BRT routes I and V share the same route, but BRT route I has a lower density of bus stations per kilometre amounting to 1.0, whereas BRT route V has got 1.7 bus stations per kilometre. In addition to different driving cycles, GPS data was used to create an elevation profile for each BRT route. The topology of a route is another influential factor on TTW energy use and exhaust emissions of road vehicles (Lajunen, 2014b; Prati et al., 2014) and was, therefore, considered in the simulations.

Both hybrid-electric and plug-in hybrid-electric powertrains in the bus models in ADVISOR were configured in parallel using a power split option, i.e. the electric motor can run either solely or simultaneously with an internal combustion engine that is used as range extender (field study information). The feature of air conditioning was switched off in the simulations to consider the same thermal comfort in all buses (field study information). It should be noted that most of the buses do not possess air conditioning in Curitiba, because the city has a relative mild climate in the South Region of Brazil.

<table>
<thead>
<tr>
<th>BRT route</th>
<th>I</th>
<th>II</th>
<th>III</th>
<th>IV</th>
<th>V</th>
<th>VI</th>
<th>VII</th>
</tr>
</thead>
<tbody>
<tr>
<td>One-way distance (km)</td>
<td>10</td>
<td>11</td>
<td>16</td>
<td>18</td>
<td>24</td>
<td>10</td>
<td>10</td>
</tr>
<tr>
<td>Number of bus stations</td>
<td>10</td>
<td>6</td>
<td>32</td>
<td>16</td>
<td>40</td>
<td>19</td>
<td>21</td>
</tr>
<tr>
<td>Number of bus stations per kilometre</td>
<td>1.0</td>
<td>0.5</td>
<td>2.0</td>
<td>0.9</td>
<td>1.7</td>
<td>1.9</td>
<td>2.1</td>
</tr>
</tbody>
</table>
The bus manufacturer of the plug-in hybrid-electric two-axle bus (PlugTwA) states a usable capacity of 8.5 kWh for the on-board battery (Volvo Group, 2015). The usable capacity states the capacity range that is actually used of the nominal capacity and is bounded by an upper limit, i.e. the high state-of-charge (SOC_high), and a lower limit, i.e. the low state-of-charge (SOC_low). The operation of the PlugTwA bus started at SOC_high in the simulations and used all-electric operation until the battery was depleted to a certain state-of-charge threshold (SOC_threshold). When the threshold was reached, the operation switched from charge-depleting mode to charge-sustaining mode. The term charge-depleting mode refers to the operation of a plug-in hybrid-electric bus when more electricity is used than being recovered from the regenerative braking system, i.e. the SOC decreases over distance or time. In comparison, the term charge-sustaining mode refers to the operation of hybrid-electric and plug-in hybrid-electric buses when the SOC maintains approximately constant due to a sustainable balance between electricity use for all-electric drive and electricity generation in the regenerative braking system. The values for SOC_low, SOC_high and SOC_threshold were based on field study information. A visualisation of charge-depleting and charge-sustaining modes is shown in Figure 6.

The charge-sustaining mode of PlugTwA represents the same operation as in the cases of the hybrid-electric buses (HybTwO, HybTwA, HybArA), i.e. regenerative braking is used to recharge the battery and all-electric operation is used up to a speed of 20 km/h based on field study information. This implies that the operation in charge-sustaining mode has a net zero energy use as only the amount of electricity is used for all-electric operation that was previously recovered by the regenerative braking system. Above a speed of 20 km/h, both electric motor and internal combustion engine run in parallel. Concerning the charge-depleting mode, i.e. electricity use between SOC_high and SOC_threshold, the bus manufacturer states an all-electric range of 7 km (Volvo Bus Corporation, 2019). This gives a TTW energy use for electricity of 3.86 MJ_TTW/km. This value is close to other estimations, e.g. by (Lajunen, 2012b) who simulated the operation of an electric bus for four different driving cycles using ADVISOR.

After creating in ADVISOR models of the buses, driving cycles and elevation profiles, the simulations were run and TTW energy use estimations obtained. Those TTW energy use estimations were then multiplied with the factors estimated for WTW fossil energy use and WTW GHG emissions from Table 1 to obtain the amounts of the respective estimates in the functional units per kilometre and passenger-kilometre.

Figure 6: Trend of the state-of-charge (SOC) in the battery for charge-depleting (CD) and charge-sustaining (CS) modes for the operation of a plug-in hybrid-electric bus over distance (modified figure from Paper II)
Results

TTW energy use, WTW fossil energy use and WTW GHG emissions were estimated for the six buses considering their operation on seven BRT routes at six operation times. The estimations from ADVISOR were validated through comparison to scientific studies as well as published real-world data from Curitiba (see Paper I for more details). The arithmetic mean values of all estimations for each bus are shown in Figure 7 for TTW energy use and in Figure 8 for both WTW fossil energy use and WTW GHG emissions. The range bars show the data spread between the minimum and maximum values for each bus considering all BRT routes and operation times.

First of all, the results show that TTW energy use of a bus depends on the BRT route and operation time as indicated by the large range bars around the mean values (Figure 7a,b). This applies to all types of buses in this analysis. On average, the hybrid-electric two-axle buses (HybTwO, HybTwA) and the plug-in hybrid-electric two-axle bus (PlugTwA) use 30% and 58% less TTW energy than the conventional two-axle bus (ConvTwO: 17.46 MJ\text{TTW}/km), respectively (Figure 7a). Obviously, an electrification of the powertrain in a bus can considerably save TTW energy in the operation phase.

While the conventional bi-articulated bus uses the most TTW energy per kilometre (ConvBiO: 29.92 MJ\text{TTW}/km), its TTW energy use per passenger-kilometre (ConvBiO: 0.22 MJ\text{TTW}/pkm) is below the values of both hybrid-electric two-axle buses (HybTwO: 0.29 MJ\text{TTW}/pkm; HybTwA: 0.24 MJ\text{TTW}/pkm) (Figure 7b). This is achieved by transporting many passengers in its large passenger carrying capacity and thus, TTW energy use per passenger-kilometre is considerably reduced. Besides, this is also the reason for the lower TTW energy per passenger-kilometre of HybTwA as its passenger carrying capacity is slightly larger in comparison to HybTwO (HybTwO: 0.29 MJ\text{TTW}/pkm, PCC: 79; HybTwA: 0.24 MJ\text{TTW}/pkm, PCC: 95).

A combination of both advanced (electrified) powertrain and large passenger carrying capacity is given in the case of the hybrid-electric articulated bus (HybArA). This combination made it possible that the bus achieved a lower TTW energy per passenger-kilometre than ConvBiO (Figure 7b), despite its smaller passenger carrying capacity (ConvBiO: 0.22 MJ\text{TTW}/pkm, PCC: 250; HybTwA: 0.18 MJ\text{TTW}/pkm, PCC: 154).

The least TTW energy use per kilometre and per passenger-kilometre were achieved by the plug-in hybrid-electric two-axle bus (PlugTwA: 7.36 MJ\text{TTW}/km, 0.14 MJ\text{TTW}/pkm). Thus, a higher degree of electrification such as in the case of the PlugTwA bus can even compete with buses having larger passenger carrying capacities (ConvBiO, HybArA) and an electrified powertrain (HybArA). This implies that an operation of the plug-in hybrid-electric bus could be of interest during operation times when the ridership is low in the BRT system, since less passengers need to be transported, and on the condition that its passenger carrying capacity is sufficient.

Figure 7: TTW energy use per kilometre (km) and passenger-kilometre (pkm) (condensed results from Paper I)
Another finding concerning TTW energy use is that the operation on BRT route I is 10–26% more energy-efficient compared to BRT route VI. Both BRT routes use the same route in Curitiba, but BRT route I has got 10 bus stations and BRT route VI has got 19 bus stations. As a result, the lower bus station density improves the flow of buses which results in higher average speeds and eventually, reduces stop-and-go operation. This all has presumably led to the observed more energy-efficient operation.

The buses ConvTwO, ConvBiO, HybTwO, HybTwA and HybArA only consume the biodiesel blend B7, whereas PlugTwA additionally uses electricity. The relative difference among the firstly mentioned five buses are the same as for the TTW energy use estimations, since their TTW energy use was multiplied with constant factors for WTW fossil energy use and WTW GHG emissions from Table 1.

The WTW fossil energy use (Figure 8a,b) and WTW GHG emissions (Figure 8c,d) estimations show that most of the WTW fossil energy is used in the operation phase due to the high fossil energy content in the biodiesel blend B7. While 16.6% of the total WTW fossil energy is used to produce and supply the biodiesel blend B7, the vast amount of WTW fossil energy (83.4%) is used due to the combustion of the petroleum diesel component in the biodiesel blend B7. Similarly, this applies to the WTW GHG emissions. The shares between WTT GHG emissions and TTW GHG emissions to the total WTW GHG emissions amount to 79.5% and 20.5%, respectively. In the case of PlugTwA, the WTT scope is more important, since less TTW energy is used in the operation phase. The WTT scope contributes to 34.0% and the TTW scope contributes to 66.0% of the total WTW fossil energy use of PlugTwA. The WTT scope is even more important than the TTW scope concerning the total WTW GHG emissions (WTT: 42.2%; TTW: 57.8%). Note: Similar shares were found by (Nylund et al., 2012) who estimated that the WTT scope accounts for 20% and the TTW scope account for 80% of the total WTW scope in the case of petroleum diesel; and 30% for the WTT scope and 70% for the TTW scope in the case of biofuels.

![Figure 8: WTW fossil energy use and WTW GHG emissions per kilometre (km) and passenger-kilometre (pkm) (condensed results from Paper I)](image-url)
The results for both WTW fossil energy use and WTW GHG emissions provide the following insights: A decarbonisation in the public bus transport system is possible when using advanced (electrified) buses compared to conventional buses due to less TTW energy use. Meanwhile, this implies that for every unit of TTW energy saved, a proportional amount of fuel does not need to be produced and supplied. Therefore, energy efficiency improvements in the operation phase also reduce effectively both WTT energy expended and WTT GHG emissions released to produce and supply fuels for the transport sector. This means that decisions concerning the choice of bus technology in the operation phase can also avoid upstream impacts in the fuel pathways. Thus, the shares indicate that the city of Curitiba and bus operators could also influence the amount of WTT fossil energy use and WTT GHG emissions when using hybrid-electric and plug-in hybrid-electric buses instead of conventional buses.

In summary, the analysis of TTW energy use, WTW fossil energy use and WTW GHG emissions showed that considerable amounts of energy and GHG emissions can be reduced when replacing conventional buses by hybrid-electric buses. Considering the advantage of hybrid-electric buses that they do not need any charging infrastructure, a significant cut of energy and GHG emissions can be already achieved. Once charging infrastructure is implemented, plug-in hybrid-electric buses can be used leading to drastic energy and GHG emissions reductions as shown when comparing the conventional buses ConvTwO or ConvBiO to the plug-in hybrid-electric bus PlugTwA. Meanwhile, the actual number of passengers, that is transported, must be considered as energy and GHG emissions can be related to them. In this regard, the simulations showed that the conventional bi-articulated bus can be more energy-efficient in terms of TTW energy use per passenger-kilometre compared to hybrid-electric two-axle buses. However, this requires to transport many passengers, otherwise its energy use of 29.92 MJTTW/km is much higher compared to any other bus in the analysis. Another interesting insight is that the biodiesel blend B7 reduces only 5.5% of WTW fossil energy use and 5.1% of WTW GHG emissions compared to pure petroleum diesel (Table 1). In this respect, much higher reductions of both WTW fossil energy use and WTW GHG emissions can be achieved by implementing a technological shift from the use of conventional powertrains to hybrid-electric powertrains in buses — resulting in a reduction of 30% TTW energy use. Lastly, all buses achieved a TTW energy use per passenger-kilometre of less than 0.5 MJTTW/pkm on average. This is an important finding as this is the numeric value suggested by the IPCC to achieve a concentration of 450 ppm (parts per million) of CO₂e in the atmosphere concerning the climate target to limit global warming to 2°C (Creutzig et al., 2015; Edenhofer et al., 2014).

### 2.2 Cost of Transport Service and Influential Factors

Following the TTW energy use, WTW fossil energy use and WTW GHG emissions estimations, Paper II analysed the cost of transport service and influential factors as presented in this section and the next Section 2.3.

A profitable transport system must often take a fare from passengers to cover the cost of the transport service. The fare is a very decisive factor on the use of a BRT system (Hensher and Li, 2012b; Hensher and Li, 2012a). Fuel cost are of particular interest for bus operators as those represent the second largest cost proportion — behind the salaries to the bus driver — of the total cost of transport service in the case of conventional bi-articulated buses in Curitiba’s BRT system (URBS, 2018a). On one hand, an intuitive solution would be to operate as few buses as possible to reduce both fuel cost and cost of transport service. On the other hand, the study by (dell’Olio et al., 2012) found that the more buses are operated, the more increases the satisfaction
of passengers due to a reduced headway. The headway is used as an indicator for service quality in transport science and measures the distance of time between two buses in operation on a bus route. This implies that the shorter the headway is, the less time passengers must wait until they can take the next bus. Thus, a short headway is desired to achieve a high passenger satisfaction and consequently, to attract more paying passengers.

More passengers result in more passenger load in buses. Consequently, more TTW energy is consumed (Ribau et al., 2015; Saxe et al., 2008; Q. Yu et al., 2016). Another factor is the driving cycle as already mentioned earlier. While driving cycles can differ between bus routes and operation times as presented in the previous section, they can also potentially differ on the same bus route during the same operation time due to varying bus driver behaviour and traffic situations. Although, both bus route and operation time are the same, the traffic situation can quickly change due to the traffic light system, etc. Moreover, fuel prices for the biodiesel blend and electricity have been varying in Brazil over time (ANP, 2018b; ANEEL, 2018). Consequently, fuel prices add operational uncertainty on the fuel cost for a bus and the cost of transport service.

For the stated reasons, the influence of the three factors — passenger load, driving cycle and fuel prices — on both fuel cost and cost of transport service is important to understand for the different buses. Only then, technological changes of both powertrain and chassis can be evaluated concerning changes in cost as well as impact of uncertainties. Based on this, Paper II investigated the three factors for the different types of buses. The implications of the technological changes are evaluated in potential scenarios in which the bus fleet composition is changed, and the cost of transport service and service quality are evaluated. The goal is to explore potential consequences that may affect the choice for buses in Curitiba’s BRT system. A bottom-up analysis is used whose consecutive steps are shown in Figure 9.

First, the TTW energy use per kilometre of buses was estimated considering different passenger loads and driving cycles. Then, the TTW energy use was multiplied with the fuel price for electricity or fuel price for biodiesel blend as well as the latter’s lower heating value (LHV) to compute the fuel cost and its uncertainty. In addition to the fuel cost, other cost data was considered from Curitiba’s BRT system to evaluate the importance of both fuel cost and uncertainty on the cost of transport service. Lastly, a scenario analysis was used to highlight the implications of the findings on a partly or completely replacement of buses on one BRT route. A simple techno-economic optimisation model was developed and used for data-driven decision-making on the bus fleet composition in the scenarios. A more detail description of steps 1, 2 and 3 is given over the next paragraphs in this section as well as for step 4 in the next Section 2.3.

The vehicle simulation tool ADVISOR was used in Paper II to estimate the TTW energy use of buses in operation, too. Four out of the six previous buses were considered (Table 2). The four buses include two buses that were used in Curitiba at the time of the study, namely the conventional bi-articulated bus (ConvBi) and the hybrid-electric two-axle bus (HybTw — previously abbreviated as HybTwO) as well as two buses that represent potential energetic and environmental alternatives, namely the hybrid-electric articulated bus (HybAr) and plug-in hybrid-electric two-axle bus (PlugTw). The biodiesel blend B7 was again considered as a fuel.
The previous presumption that the TTW energy use of electricity for PlugTw amounts to 3.86 MJ$_{TTW}$/km was not applied in Paper II. Instead, the all-electric operation was modelled with ADVISOR to obtain a more comprehensive understanding of electricity use in PlugTw as a function of passenger load and driving cycle.

The influence of the passenger load on the TTW energy use of the buses was estimated by simulating each driving cycle for six different passenger loads that incrementally increased by 20% of the passenger carrying capacity, i.e. the passenger load was ranging from an occupancy rate of 0% (no passengers) to 100% (max. number of passengers corresponding to the passenger carrying capacity of a bus) in the simulations. To compute the vehicle mass according to the occupancy rate, the total weight of a bus at 100% passenger load was assumed to correspond to the permitted gross vehicle weight (GVW). This implies that the GVW minus the maximum aggregated passenger weight gives the total weight of an empty bus at 0% passenger load. Linear interpolation provides the remaining weights for passenger loads at 20%, 40%, 60% and 80%. The weight of one passenger was assumed to amount to 67 kg.

The BRT route, that was considered this analysis, is the previous BRT route IV or more specifically, BRT route 503 in Curitiba. This BRT route has a one-way distance of 10 km, over which 19 bus stations are distributed. Real-world bus operation data was used from eleven conventional bi-articulated buses that drove on that BRT route (URBS 2015a). The operation took place between the bus station Tubo Praça Carlos Gomes located in the north to bus station Terminal Boqueirão located in the south (Figure 10a). The operation followed the regular timetable on a weekday in the morning. In addition to the driving cycles, the elevation profile was considered, too (Figure 10b). The speed distribution of the eleven driving cycles shows that the buses drove more than 50% of their operation time above a speed of 20 km/h and reached a top speed of 55–65 km/h (Figure 10c).

In addition to passenger load and driving cycle, fuel prices such as for the biodiesel blend and/or electricity directly influence the fuel cost and cost of transport service. As the fuel cost were empirically derived from TTW energy use and fuel price data, a potential influence of the fuel prices on the operation (i.e. the dataset of the driving cycles) and likewise, on the TTW energy use was outside the scope of this analysis.

US dollar (USD) is used as monetary unit. The conversion of the local fuel prices in Brazilian Real (BRL) was done with a currency exchange rate of 0.2833 USD/BRL based on the weighted mean for values during the period from 1 January 2014 to 31 December 2017 (X-rates, 2018).
This systematic conversion between BRL and USD eliminated random uncertainty from any potential fluctuation of the exchange rate. The fuel prices (mean ± sample standard deviation) of the biodiesel blend and electricity increased over the considered period and amounted to $(0.913 \pm 0.052)$ USD/L and $(0.160 \pm 0.029)$ USD/kWh, respectively (Figure 11).

Normality tests indicate that the values of the fuel prices are not normally distributed for the considered period, which was found by analysing the data with histogram plots in the statistic software Past 3.x (Hammer et al., 2001). As a result, Chebyshev’s inequality was used to interpret the spread of data concerning both uncertainty and probability distribution. Chebyshev’s inequality follows the empirical rule that a $1 - 1/k^2$ proportion of the data is covered by $k$ standard deviations, e.g. $k = \sqrt{2}; 1 - 1/\sqrt{2}^2 = 1 - 0.5 = 0.5 = 50\%$, $k = 2; 1 - 1/2^2 = 1 - 0.25 = 0.75 = 75\%$, or $k = 3; 1 - 1/3^2 = 1 - 0.111 = 0.889 = 88.9\%$. No insights are generated in the case of one standard deviation $k = 1$ as this gives mathematically 0%. In comparison, data drawn from a normal distribution follows the empirical 68–95–99.7 rule that 68%, 95% or 99.7% of the expected values of the data are not further away from the mean than one, two or three standard deviations, respectively.
Thus, an interpretation based on Chebyshev's inequality is more conservative, because it presumes that fewer of the expected values of the data are covered by the same number of standard deviations in comparison to a normal distribution, e.g. two standard deviations cover 50% of expected values according to Chebyshev's inequality, whereas 95% of expected values would be covered according to the normal distribution.

The fuel cost of a bus was calculated by summing up the costs for biodiesel blend B7 and electricity and relating them to the functional unit of one kilometre.

The combined uncertainty of both fluctuating fuel prices and varying driving cycles on the fuel cost was estimated by calculating their combined standard uncertainty for non-linear combinations of input estimates considering their associated standard uncertainties based on the methodology by (JCGM, 2008). The input estimates were the fuel price of biodiesel blend B7, TTW energy use of biodiesel blend B7, fuel price of electricity, TTW energy use of electricity and driven distance. The standard uncertainties of those were estimated by the sample standard deviations of their measurements. More details and equations are provided in Paper II.

Uncertainties are described by the coefficient of variation (CV), which measures the relative dispersion of values around the mean, i.e. uncertainty — the sample standard deviation — divided by the mean. In the case of fuel prices, the CV for the fuel price of the biodiesel blend and electricity amounted to 6.2% and 18.2% over the considered period, respectively.

The cost of transport service was calculated for each bus based on its fuel cost, as estimated from the TTW energy use simulations and fuel price data, and other cost components based on real-world data from Curitiba’s bus transport system. The cost of transport service represents the total cost that needs to be covered by the fare to operate the bus transport system in a profitable manner in Curitiba. The other cost components are the technical operating cost of the bus fleet, personnel cost, administration cost, amortisation of buses and facilities, profitability requirements, taxes and some small cost addition to account for the amortisation and profitability requirements of investments made for the renewal of the bus fleet between 2013 and 2016 (URBS, 2017). A compilation of cost data was available online that was published by Curitiba’s public bus transport authority URBS (URBS, 2018a). Moreover, URBS published their applied calculation methodology for the fare. Altogether, i.e. the cost data and methodology, provided transparency and made an alignment of all calculations in Paper II possible to the local requirements. Since the conventional bi-articulated bus (ConvBi) and hybrid-electric two-axle bus (HybTw) had been already operated in Curitiba, their cost data was completely available
online. The remaining two buses in the analysis were only in a test phase at the time of the research and hence, not all cost data was available for those. Therefore, some assumptions were made based on observations in the real-world cost dataset from Curitiba. A full overview on all cost data and assumptions is given in Paper II.

Results

TTW energy use was estimated for the four buses based on simulations for six passenger loads and eleven driving cycles, i.e. 66 simulations per bus or 264 simulations in total for all buses. The estimations from ADVISOR were validated through comparison to scientific studies as well as published real-world data from Curitiba (see Paper II for more details). The TTW energy use estimations were used to calculate the cost of transport service.

The TTW energy use values are normally distributed based on the Shapiro-Wilk test in Past 3.x (Hammer et al., 2001) as well as considering that skewness and kurtosis were within a range of ±2 for the values in the data distribution. This observations further imply a normal distribution for driving cycles and their influence on the TTW energy use.

The TTW energy use trends over the passenger load are shown in Figure 12a. The by far largest and widest TTW energy use range was estimated for the conventional bi-articulated bus ConvBi (24.89—36.50) MJTTW/km due to its heavy chassis and energy-inefficient conventional powertrain when compared to the three advanced buses. Less energy is used by the two hybrid-electric buses (HybTw: 11.51–14.20 MJTTW/km; HybAr: 13.45–16.91 MJTTW/km). The lowest TTW energy use is observed for the plug-in hybrid-electric bus PlugTw (6.24–10.33 MJTTW/km). Furthermore, the simulations showed that this bus uses 63% less TTW energy in charging-depleting mode than in charge-sustaining mode. Thus, all-electric operation is much more energy-efficient than charge-sustaining operation due to avoidance of any liquid fuel combustion in an internal combustion engine.

Another observation is the sensitivity of TTW energy use to passenger load changes. Measured in absolute change, the most sensitive bus is ConvBi, for which the TTW energy use increases by 0.46 MJTTW/km (1.9%) for every incremental increase of 10 passengers — on average considering the mean value from the lowest TTW energy use value at a passenger load of 0% and the highest TTW energy use value at a passenger load of 100%, related to the passenger carrying capacity of a bus. In comparison, the TTW energy use increases by 0.34 MJTTW/km (3.0%) for HybTw, 0.23 MJTTW/km (1.7%) for HybAr and 0.17 MJTTW/km (4.2%) for PlugTw in charge-depleting mode or 0.41 MJTTW/km (3.7%) for PlugTw in charge-sustaining mode considering the same incremental increase. These observations imply that advanced buses with increasing degree of electrification are less influenced by passenger load changes than conventional buses — concerning an absolute change of TTW energy use.

Figure 12b shows drastically decreasing trends for the TTW energy use per passenger-kilometre for all buses, i.e. the TTW energy use increases slower than linear to a passenger load increase in terms of number of passengers. Thus, despite an increasing TTW energy use per kilometre, the number of passengers transported in a bus should be increased, because consequently, the TTW energy use per passenger-kilometre decreases. This insight supports the recommendations from the previous analysis that it is more energy-effective to transport as many passengers as possible in a bus to achieve a low TTW energy use per passenger-kilometre.

The magnitude of the influence of varying driving cycles on the TTW energy use is different for each bus and can be categorised by type of powertrain. The influence increases with increasing degree of electrification in the powertrain.
ConvBi is the least influenced by varying driving cycles (CV: 4–5%), followed by HybTw and HybAr (CV: 8–9%) and PlugTw (CV: 13–16%). However, measured in absolute change, this operational uncertainty causes an absolute standard deviation of 1.17–1.62 MJTTW/km for ConvBi over its possible passenger load range, followed by HybAr (1.09–1.41 MJTTW/km), PlugTw (1.01–1.36 MJTTW/km) and HybTw (0.95–1.30 MJTTW/km). Consequently, while ConvBi is the least sensitive to varying driving cycles concerning a relative change, this bus shows the largest standard deviation for TTW energy use concerning an absolute change. Based on this, the operation of this conventional bus adds the most absolute uncertainty to bus operators concerning TTW energy use, whereas the advanced buses add the least absolute uncertainty. Nevertheless, the advanced buses show the largest relative standard deviation, i.e. CV value, and thus, the influential factor of varying driving cycle should be considered in their economic review, since larger relative deviation are possible in comparison to the conventional bus ConvBi.

Moreover, while PlugTw revealed the strongest relative sensitivity to varying driving cycles, the effect decreases with increasing passenger load, i.e. from a CV of 16% at zero passenger load to a CV of 13% at a maximum passenger load. The reason for the opposite trend originates from the share between charging-depleting mode and charging-sustaining mode. At higher passenger loads, more TTW energy is needed for PlugTw’s propulsion. The consequence is a more rapid depletion of its battery and as a result, an earlier start of charge-sustaining mode. The latter consumes more energy in form of biodiesel blend B7 in the internal combustion engine. Eventually, this gives a lower overall energy efficiency. The more charge-sustaining operation is used and likewise, the less charge-depleting operation, the more PlugTw operates like hybrid-electric buses then. Eventually, this leads to similar uncertainty levels for the plug-in hybrid-electric bus PlugTw in comparison to the hybrid-electric buses HybTw and HybAr.

The fuel cost is lesser important for the cost of transport service with increasing degree of electrification in the powertrain in a bus. For example, the fuel cost represents 19.7% of the cost of transport service for the conventional bus ConvBi, followed by the two hybrid-electric buses (HybTw: 10.9%; HybAr: 9.7%), and lastly, the plug-in hybrid-electric bus (PlugTw: 8.1%). The trend is expected as the absolute TTW energy use decreases with increasing degree of electrification. Regarding uncertainty, the combined standard uncertainty is consistently higher by 2–3%-point than the uncertainty due to only varying driving cycle, as uncertainty due to fluctuating fuel prices is added. The CV, considering the combined uncertainty, increases for ConvBi from 4.8% (only uncertainty due to varying driving cycles) to 7.9% (combined uncertainty
due to varying driving cycles and fluctuating fuel prices). Similarly, the CV increases from 8.9% to 11.0% for HybTw; from 8.5% to 10.6% for HybAr; and from 13.7% to 15.6% for PlugTw. As ConvBi has the highest absolute TTW energy use, its CV for fuel cost also increases the most compared to the advanced buses. The CV increases the least for PlugTw despite its two external energy sources — biodiesel blend B7 and electricity. Thus, PlugTw’s charge-depleting operation reduces TTW energy use as well as mitigates absolute uncertainty effects caused by fluctuating fuel prices.

For more statements on the distribution of data around the previously stated mean values, Chebyshev’s inequality was applied to quantify the extent of deviation for the case of $k = 3$, i.e. three standard deviations are expected to cover 88.9% of the expected values around the mean. This gives a value for $3 \cdot CV$ of 24% for ConvBi; 33% for HybTw; 32% for HybAr; and 47% for PlugTw. The multiple consideration of relative uncertainty also shows that the higher relative uncertainty for advanced buses increases even more when aiming at a coverage of 88.9% of potential values. Nevertheless, the same as before applies, i.e. the multiple of the absolute standard deviation for advanced buses is still smaller than for the conventional bus.

A summary of the insights from the sensitivity analysis of varying passenger load and uncertainty analyses of varying driving cycles and/or fluctuating fuel prices is provided in Table 4. The compiled results present a relative assessment between the bus technologies concerning the importance of the analysed influential factors in terms of absolute change and relative change. A relative grading is applied among the buses using the following grades: high impact (H), medium impact (M) and low impact (L).

For example, the largest absolute change in TTW energy use to passenger load changes was found for ConvBi in comparison to the remaining buses, and therefore, this bus is graded with the relative grade H.

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<th>Change</th>
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<th>Uncertainty from varying driving cycles on TTW energy use</th>
<th>Uncertainty from fluctuating fuel prices on fuel cost</th>
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</tbody>
</table>
In comparison, PlugTw was the least influenced by varying passenger load concerning absolute changes of TTW energy use and therefore, it is graded with the relative grade L. The hybrid-electric buses as well as the charge-sustaining operation of the plug-in hybrid-electric bus are situated in-between and graded with the relative grade M. Based on the compiled insights and relative assessment, it can be concluded that advanced buses can reduce operational uncertainty concerning an absolute variation of TTW energy use and fuel cost for bus operators.

### 2.3 Evaluation of Scenarios

Scenarios for partly or complete replacements in the bus fleet were analysed to evaluate the implications of the previous findings. The evaluation was based on two measures: cost of transport service per week and average headway in minutes per bus. The headway is the inverse of frequency (buses/hour) and states the distance of time between buses on average over one week of operation. The smaller the headway is, the shorter passengers must wait for the next bus at a bus station and as the better the service quality can be considered.

A simple techno-economic linear optimisation model was developed and used to determine the bus fleet compositions in the scenarios. The objective of the optimisation model was to minimise the cost of transport service per week. The baseline scenario represents the current situation based on the number of conventional bi-articulated buses operating on BRT route 503 in Curitiba (ScBaseline). The information was collected from the timetable that was published online (URBS, 2018c). Additionally, some alternative scenarios were considered to evaluate deployments of hybrid-electric and plug-in hybrid-electric buses (HybTw, HybAr, PlugTw) as summarised in Table 5. Minimum and maximum targets were added as constraints to the optimisation model to ensure the correct deployment of buses in the respective scenarios. Moreover, another constraint was added to consider that at least the same aggregated passenger carrying capacity has to be provided by the buses on an hourly basis as in the baseline scenario. This constraint ensured that the bus fleets in the scenarios were not undersized.

A short note regarding PlugTw: The optimisation model only focused on bus technologies and associated costs, but not on any charging requirements for this bus.

### Table 5: Baseline and alternative scenarios (modified table from Paper II)

<table>
<thead>
<tr>
<th>Scenario</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>ScBaseline</td>
<td>This scenario represents the current situation, in which only conventional bi-articulated buses (ConvBi) are operated.</td>
</tr>
<tr>
<td>ScConv50</td>
<td>This scenario represents the potential situation, in which maximal 50% of the buses in the bus fleet are conventional bi-articulated buses (ConvBi).</td>
</tr>
<tr>
<td>ScConv0</td>
<td>This scenario represents the potential situation, in which no conventional bi-articulated buses (ConvBi) are operated, i.e. complete replacement by any of the other types of buses.</td>
</tr>
<tr>
<td>ScHybrid100</td>
<td>This scenario represents the potential situation, in which all conventional bi-articulated buses (ConvBi) are replaced by only hybrid-electric buses, such as by hybrid-electric two-axle buses (HybTw) and/or by hybrid-electric articulated buses (HybAr).</td>
</tr>
<tr>
<td>ScPlug25</td>
<td>This scenario represents the potential situation, in which all conventional bi-articulated buses (ConvBi) are replaced and by at least 25% plug-in hybrid-electric two-axle buses (PlugTw).</td>
</tr>
<tr>
<td>ScPlug50</td>
<td>This scenario represents the potential situation, in which all conventional bi-articulated buses (ConvBi) are replaced and by at least 50% plug-in hybrid-electric two-axle buses (PlugTw).</td>
</tr>
<tr>
<td>ScPlug100</td>
<td>This scenario represents the potential situation, in which all (100%) buses in the bus fleet must be plug-in hybrid-electric two-axle buses (PlugTw).</td>
</tr>
</tbody>
</table>
Results

Changes in the cost of transport service per week, frequency of buses, average headway and change of waiting time for passengers are shown for the baseline and alternative scenarios in Table 6. Note: The bus fleet compositions in the scenarios are presented as shares in percent, whereas the actual number of buses by bus technology type were determined using integers in the optimisation model — logically, because only complete buses can be used in the real world.

The cost of transport service per week amounts to 61 000 USD in the baseline scenario (ScBaseline) to operate exclusively conventional bi-articulated buses with an average headway of 11.0 minutes. All other scenarios have higher cost of transport service per week. Meanwhile, the service quality increases in those scenarios, too.

For example, if at least half of the conventional buses are replaced by advanced buses, then the cost of transport service per week increases by 30%. At the same time, the waiting time is reduced by 26%. The bus fleet composition in the ScConv50 scenario shows that 40% of the conventional buses are replaced by HybAr due to its relatively large passenger carrying capacity (PCC: 154) when compared to HybTw (PCC: 79) or PlugTw (PCC: 96). The remaining bus fleet consists of 12% HybTw and 1.6% PlugTw. The share of 1.6% of PlugTw is an interesting finding as it shows that this bus can compete with HybTw despite its higher cost of transport service per kilometre (PlugTw: 3.716 USD/km; HybTw: 3.049 USD/km). The reason is that PlugTw’s passenger carrying capacity amounts to 96 passengers, which is significantly more than for HybTw (PCC: 79). Based on this observation, it can be stated that the cost of transport service per kilometre is not the only decisive criterion for the techno-economic competitiveness of a bus technology, but also its passenger carrying capacity.

The next two scenarios ScConv0 and ScHybrid100 have the goal to achieve a complete replacement of the conventional bi-articulated buses. The findings in the ScConv0 scenario reinforce the previous insights from the ScConv50 scenario, i.e. HybAr represents the most competitive techno-economic option. Nevertheless, PlugTw’s share increased to 5.3% in the ScConv0 scenario, which is only slightly lesser than for HybTw (6.5%). The remaining three scenarios ScPlug25, ScPlug50 and ScPlug100 have the goal to introduce more electrification on BRT route 503 in Curitiba and require a minimum share of plug-in hybrid-electric buses of 25%, 50% and 100%, respectively. Neither of those scenarios deploy any HybTw buses. Interestingly, despite the requirement of a minimum share of 25% for PlugTw in the ScPlug25 scenario, this bus technology reached a share of 40.9%. This reinforces the previous insight that, based on techno-economic aspects, PlugTw can compete with HybTw. If only compared by economic aspects, only the cost of transport service would be considered. Thus, the cheapest technology would be always chosen. Otherwise, the hybrid-electric articulated bus HybAr is used to complement the plug-in hybrid-electric buses PlugTw.

Considering the trends in all scenarios, a trade-off is observable between the cost of transport service per week and service quality in terms of average headway. While the cost of transport service per week increases by at least 30% up to 139% in the scenarios, the service quality also increases as measured by the decreasing average headway from 11 minutes in the baseline scenario down to 4 minutes in the ScPlug100 scenario.
Table 6: Cost of transport service (CTS) and service quality measures in the baseline and alternative scenarios (modified table from Paper II)

<table>
<thead>
<tr>
<th>Scenario</th>
<th>CTS per week change (%)</th>
<th>Frequency (buses/hour)</th>
<th>Average headway (minutes/bus)</th>
<th>Waiting time change (%)</th>
<th>Bus fleet composition (%)</th>
</tr>
</thead>
<tbody>
<tr>
<td>ScBaseline</td>
<td>0</td>
<td>5.4</td>
<td>11.0</td>
<td>0</td>
<td>100</td>
</tr>
<tr>
<td>ScConv50</td>
<td>30</td>
<td>7.4</td>
<td>8.1</td>
<td>-26</td>
<td>46.4</td>
</tr>
<tr>
<td>ScConv0</td>
<td>64</td>
<td>9.4</td>
<td>6.4</td>
<td>-42</td>
<td>0</td>
</tr>
<tr>
<td>ScHybrid100</td>
<td>64</td>
<td>9.4</td>
<td>6.4</td>
<td>-42</td>
<td>0</td>
</tr>
<tr>
<td>ScPlug25</td>
<td>80</td>
<td>10.5</td>
<td>5.7</td>
<td>-48</td>
<td>0</td>
</tr>
<tr>
<td>ScPlug50</td>
<td>85</td>
<td>10.9</td>
<td>5.5</td>
<td>-50</td>
<td>0</td>
</tr>
<tr>
<td>ScPlug100</td>
<td>139</td>
<td>14.8</td>
<td>4.0</td>
<td>-64</td>
<td>0</td>
</tr>
</tbody>
</table>

Recap of chapter 2

This chapter presented estimations for Tank-to-Wheel (TTW) energy use, Well-to-Wheel (WTT) fossil energy use, WTT GHG emissions, fuel cost, cost of transport service, sensitivity and uncertainty. Moreover, scenarios were evaluated to highlight implications of changing the composition of the bus fleet on the cost of transport service and service quality. The simulation tool Advanced Vehicle Simulator (ADVISOR) was used to create detailed vehicle models of the buses consisting of different types of powertrains and chassis, i.e. bus technologies. Real-world bus operation data from the Bus Rapid Transit (BRT) system in Curitiba was used to consider both local real-world driving cycles and elevation profiles.

The analysis estimated large potentials to save energy and reduce GHG emissions during the operation phase of the buses (TTW scope), e.g. TTW energy savings of 30% and 58% when using hybrid-electric or plug-in hybrid-electric buses compared to conventional buses having a two-axle chassis. The buses used less than 0.5 MJ/ pkm on average, which is the numeric value suggested by the IPCC to achieve a concentration of 450 ppm of CO₂e in the atmosphere concerning the climate target to limit global warming to 2°C (Creutzig et al., 2015; Edenhofer et al., 2014). Since TTW energy use also avoids fuel production and supply (WTT scope), the benefits on the WTT scope are even larger. Hybrid-electric two-axle buses can save 30% of both TTW fossil energy use and WTT GHG emissions, and the plug-in hybrid-electric two-axle bus can save 75% of TTW fossil energy use and can reduce 72% of WTT GHG emissions. Thus, the replacement of conventional buses by advanced buses for operation also contributes to the avoidance energy expended and emissions released to produce and supply fuels.

The passenger load was identified as a very influential factor for all types of buses. The largest absolute change in TTW energy use to passenger load changes was found for the conventional bi-articulated bus. In comparison, the plug-in hybrid-electric two-axle bus was the least influenced by varying passenger load concerning absolute changes of TTW energy use. The hybrid-electric buses as well as the charge-sustaining operation of the plug-in hybrid-electric bus are situated in-between. The analysis of uncertainty, caused by varying driving cycles and fluctuating fuel prices, again showed that the fuel cost of conventional bi-articulated bus is influenced the most due to its considerable TTW energy use. Based on the complied insights and relative assessment, it can be concluded that advanced (electrified) buses can reduce uncertainty concerning an absolute variation of TTW energy use and fuel cost for bus operators.
The scenarios highlighted the implications on the cost of transport service per week and average headway on the BRT route 503 in Curitiba. Considering the trends in all scenarios, a trade-off was observed between cost of transport service per week and service quality in terms of average headway. While the cost of transport service per week increased by at least 30% up to 139% in the alternative scenarios compared to the current situation, in which only conventional bi-articulated buses are operated, the service quality also increased as measured by the decreasing average headway from 11 minutes down to 4 minutes in the scenario in which only plug-in hybrid-electric buses are operated.
3 MANAGEMENT STRATEGIES FOR AN ELECTRIFIED BUS FLEET

This third chapter analyses management strategies for a plug-in hybrid-electric bus fleet in operation. A real-time optimisation model was developed and tested to estimate operational optimisation potentials for energy savings and all-electric operation. Several scenarios are evaluated for a subsystem of Curitiba’s BRT system. The research presented in this chapter is based on scientific paper III (referenced as Paper III).

3.1 REAL-TIME OPTIMISATION MODEL

Proof-of-concept projects usually implement one fast charging station to provide opportunity charging to one or a few plug-in hybrid-electric buses in the real world, e.g. as tested in Curitiba (Automotive World, 2016). Furthermore, those buses usually operate on only one bus route and the distance of time between buses is usually enough for smooth charging. However, the situation becomes more challenging when scaling-up. In that case, an increasing number of buses needs to be recharged and potentially at the same charging station at the same time. For example, this situation can occur when several bus routes share the same charging station. Decisions must be made for the charging schedule then. Those shall ensure charging without any delays or partial gridlocks of the transport service. Such decisions are defined as a management strategy in the following case study.

Plug-in hybrid-electric buses are of particular interest, since the duration of their all-electric operation depends on the possibility to recharge their on-board batteries. If no recharging is possible and the battery in a bus is depleted, an internal combustion engine is used as range extender then. The range extender still ensures reliable operation and punctuality of the transport service. However, it conflicts with utilising available potentials to reduce TTW energy use as well as global and local emissions. Hence, the operational management of plug-in hybrid-electric buses is crucial to unlock the potential of this bus technology.

An intuitive management strategy to allocate buses to charging stations can be implemented according to the buses’ arrival times at a bus station that is equipped with a charging station, i.e. management strategy A: prioritise buses for charging by arrival times at the charging station (first come, first served). This management strategy is commonly applied when only a few plug-in hybrid-electric buses are operated, and no conflict is expected.

The all-electric operation of plug-in hybrid-electric buses is another operational aspect that can be managed. All-electric operation is usually used when enough electricity is available in the case of plug-in hybrid-electric buses. Another consideration could be to save some electricity and use it in certain areas, e.g. near hospitals to ensure a quiet environment. In any case, the all-electric operation can be managed differently depending on the strategy and target, i.e. considerations at the bus fleet management level.

Therefore, in addition to management strategy A, other management strategies are considered, such as B: prioritise buses for charging by energy intensity of the bus routes; C: minimise the total energy use of the bus fleet; D: Maximise the total all-electric time of the bus fleet; and E: Maximise the total all-electric distance of the bus fleet. Overall, the five management strategies shall ensure to allocate buses to charging stations; decide on the charge time for each bus; or additionally,
aim to minimise the total amount of TTW energy use or maximise the total all-electric operation of the bus fleet.

Proof-of-concept projects in cities can develop at different paces. This should be also considered concerning the technical implementation of management strategies. In this regard, flexibility and scalability are requirements for a technical solution. Moreover, a dynamic method is needed that can react on operational uncertainty from real-world behaviour, including the consideration of deviations from the timetable caused by unexpected events such as accidents or congestion. Considering these requirements, periodic exchange of information is needed between the buses and a control unit from which control signals are given to manage the buses.

The periodic exchange of data and use in an optimisation model refers to the control technique of real-time optimisation (RTO) (Sánchez-Martínez, 2015). Moreover, the exchange of information between objects is linked to the Internet-of-Things (IoT) concept. This popularised paradigm uses internet connectivity to collect and exchange information between objects, for example, between buses and an online platform. Real-time data about the GPS positions and batteries’ state-of-charges are sent from the buses via the internet to an IoT-platform. There, the data is stored, potentially analysed and potentially used in an optimisation model to determine an optimal solution for the charging schedule and all-electric operation for each bus ahead of time and subject to operational uncertainty. Finally, the decision signals are sent to the buses that act accordingly. The conceptual framework for the interaction between an online IoT-platform and a plug-in hybrid-electric bus fleet is illustrated in Figure 13.

An RTO model was developed to test this concept and compare the potential gains from the five management strategies A–E. The optimisation model was designed as mixed-binary linear programming problem with deterministic behaviour. The RTO model’s algebraic formulation is provided in Paper III. In this thesis, a high-level description is provided to summarise its behaviour and considerations for the case study.

**Figure 13**: Conceptual framework for the interaction between an IoT-online platform and a plug-in hybrid-electric bus fleet. C1, C2 and C3 are charging stations (formatted figure from Paper III).
The optimisation model is constructed and solved in periodic repetitions for a defined time interval, e.g. every three minutes as used in this case study for Curitiba. This implies that the optimisation model determines every three minutes optimal solutions based on available information. The time interval of three minutes is further split into smaller time steps depending on data quality and computational power, e.g. 10 s. At the time of the model’s construction, all data is collected, such as current GPS positions of the buses, current SOCs in the batteries in the buses and the expected TTW energy uses of the buses during each time step over the time interval subject to optimisation. The dataset is then provided to the optimisation model and an optimal solution is determined.

The algorithmic paradigm of this approach is a so-called Greedy algorithm, i.e. an optimal solution is determined at the time point at which the time interval starts that is subject to optimisation. In other words, the best possible solution is determined for a problem at present without consideration of any consequences after the time interval. This approach stands in contrast to finding a global optimal solution, e.g. to develop a charging schedule based the ideal timetable of a bus transport system considering an entire operation day. RTO and the Greedy algorithm approach make it is possible to consider real-time bus operation data and potentially occurring operational uncertainty in the execution of a management strategy for a plug-in hybrid-electric bus fleet in operation.

The most important decision variables in the developed model are two binary variables that are indexed for each bus and each time step. One variable is used for the decision whether a bus is charged during a time step or not; and the other variable is used for the decision whether a bus shall drive all-electric or not. One challenge to use the optimisation model is that information is needed about the future operation over the duration of the time interval. In this case study, simulations and historical bus operation data were used. Thus, the future operation data for each time interval had been known at each time point when each time interval started. Since the goal was to estimate potentials for energy savings and all-electric operation from the different management strategies, it can be argued that it was valid to use historical data and presume knowledge of future operation data.

### 3.2 Energy Savings and All-Electric Operation from Management Strategies

Hybrid-electric and plug-in hybrid-electric bi-articulated buses are in their development and implementation at an early stage (ZeEUS project, 2016). In comparison, conventional bi-articulated buses are frequently used, and particularly in BRT systems. This is also the case in Curitiba’s BRT system — the business-as-usual (BAU) scenario in the case study. Therefore, bus operation data from those buses was used in the simulations to generate insights about energy savings gained from increased electrification in a hybrid-electric bus fleet (HYB) scenario as well as plug-in hybrid-electric bus fleet (PLUG) scenario, i.e. insights at the bus technology level. The PLUG scenarios were further used to demonstrate the application of the RTO model and compare the potentials for energy savings and all-electric operation from the five management strategies A–E, i.e. insights at the bus fleet management level.

An overview on the seven scenarios and associated management strategies is given in Table 7. In summary, the BAU scenario simulates only conventional bi-articulated buses. Only diesel is used as an external energy source. The BAU scenario represents the situation in Curitiba as of now. The HYB scenario simulates the theoretical operation of hybrid-electric bi-articulated buses. Only diesel is used as an external energy source. All electricity, used in the electric motor,
is only internally generated by the on-board regenerative braking system from braking energy, i.e. zero net energy use for electricity use.

And the PLUG scenario simulates the theoretical operation of plug-in hybrid-electric bi-articulated buses. Both diesel and electricity are used as external energy sources. External electricity is provided through opportunity charging and overnight charging in a bus depot. In addition, a regenerative braking system is used to generated internally electricity.

Curitiba’s BRT system consists of nine BRT routes. Two types of bus stations exist — tube stations and terminal stations. While tube stations are like ordinary bus stations, terminal stations are large transport hubs. Three reasons make terminal stations to interesting locations to implement charging stations there: 1) terminal stations have a large spatial dimension, which gives flexibility in finding a suitable place for a charging station, 2) terminal stations are shared by many bus routes and BRT routes, which can potentially give a high utilisation rate for a charging station, 3) terminal stations are often located at the beginning and end of BRT routes, which can potentially give some more time to recharge the batteries. Based on these reasons, terminals were assumed to be suitable bus stations for charging stations in this case study. Besides, the same consideration was also used in a scientific study carried out by local researchers in Curitiba (Sebastiani et al., 2016).

To reduce computational hardware and software requirements, a subsystem of the BRT system was selected based on two criteria: 1) three BRT routes should use at least the same terminal station; and 2) two or more BRT buses should be at least 70% of the operation time at the same terminal station at the same time so that a decision must be provided by the RTO model to allocate buses. The two criteria were tested for bus operation data from the 31 October 2017. The test was only passed by terminal station Capão Raso. This terminal station is used by four BRT routes: 203, 502, 602 and 603. Thus, the systems boundary in the case study comprises one terminal station and four BRT routes (Figure 14).

Table 7: Bus technology deployment and management strategy scenarios (modified table from Paper III)

<table>
<thead>
<tr>
<th>Nº</th>
<th>Scenario</th>
<th>Management strategy</th>
<th>Powertrain technology</th>
<th>Objective</th>
<th>Optimisation target/s</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>BAU</td>
<td>-</td>
<td>Conventional</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>2</td>
<td>HYB</td>
<td>-</td>
<td>Hybrid-electric</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>3</td>
<td>PLUG-A</td>
<td>A</td>
<td>Plug-in hybrid-electric</td>
<td>Prioritise buses for charging by arrival times at the charging station</td>
<td>Charging schedule</td>
</tr>
<tr>
<td>4</td>
<td>PLUG-B</td>
<td>B</td>
<td>Plug-in hybrid-electric</td>
<td>Prioritise buses for charging by energy intensity of the bus routes</td>
<td>Charging schedule</td>
</tr>
<tr>
<td>5</td>
<td>PLUG-C</td>
<td>C</td>
<td>Plug-in hybrid-electric</td>
<td>Minimise total energy use of the bus fleet</td>
<td>Charging schedule and all-electric operation</td>
</tr>
<tr>
<td>6</td>
<td>PLUG-D</td>
<td>D</td>
<td>Plug-in hybrid-electric</td>
<td>Maximise total all-electric time of the bus fleet</td>
<td>Charging schedule and all-electric operation</td>
</tr>
<tr>
<td>7</td>
<td>PLUG-E</td>
<td>E</td>
<td>Plug-in hybrid-electric</td>
<td>Maximise total all-electric distance of the bus fleet</td>
<td>Charging schedule and all-electric operation</td>
</tr>
</tbody>
</table>
The subsystem was simulated with two weeks of bus operation data collected from conventional buses in Curitiba’s BRT system during the period 8–21 January 2018 (UFPR, 2019). By using the real-world bus operation data from conventional buses, the data implies the requirement to maintain the same punctuality and transport service in the BRT system also in the scenarios when simulating the operation of hybrid-electric or plug-in hybrid-electric buses. Both BAU and HYB scenarios did not use the RTO model. Those served as scenarios for comparison and measurement of energy savings and all-electric operation with increasing degree of electrification. Thus, the RTO model was only applied in the PLUG scenarios considering the five management strategies A–E.

Some data preparation was needed to test the RTO model. The dataset of one operation day was split into three-minute chunks of data that consecutively built one operation day. The chunks of the dataset consisted of several data points and each data point contained information about the buses’ identification number, GPS coordinates and time stamp. However, information about the TTW energy use of the buses was not provided. Moreover, no data about the SOC was available as the bus operation data originated from conventional buses. Hence, some additional calculations and assumptions were needed to complement the dataset and to provide the required input data to the RTO model. First, the initial SOCs were assumed to be at 85%, i.e. the level of electricity in the buses’ batteries at operation start. Next, the TTW energy use was estimated for: 1) operation only with the electric motor, i.e. all TTW energy use from the battery to the wheels; 2) operation only with the internal combustion engine, i.e. all TTW energy use from the fuel tank to the wheels; 3) regenerative braking, i.e. all energy recovery from the braking energy at the wheels to the battery.

Exact estimations are analytically impossible due to the complexity and non-linearities in the powertrain components as well as their interplay. While some simulation tools, e.g. ADVISOR as used in Paper I and Paper II, can estimate TTW energy use values quite accurately, such an advanced simulation tool was not suitable in this case study due to the much larger amount of bus operation data compared to the case studies in Paper I and Paper II. Moreover, TTW energy use was required to be calculated from route-specific and time-specific driving cycles to overcome
those limitations as found in other scientific studies. Based on these requirements, a backwards-calculating energy use rate estimation method was used for each bus and each data point. The method is backwards-calculating, because calculations are made opposite to the actual energy flow direction, i.e. not from the fuel tank or battery to the wheels, but from the wheels to the fuel tank or battery.

The method starts with accounting of the occurring forces from the driving cycle and elevation profile on a bus. The forces include air resistance, gradient force, rolling resistance and the directional force. From those, the instantaneous power demand at the wheels of a bus is calculated. In an ideal world, the instantaneous power demand at the wheels would be the same as the energy use rate from the fuel tank or battery, i.e. no losses would exist. However, losses occur in the powertrain components and therefore, those needed to be accounted, too. Since ADVISOR was not suitable here, constant values for the powertrain efficiencies were assumed based on literature and own calculations, namely a TTW energy efficiency for the operation with the internal combustion engine of 25% (Nylund et al., 2007); a TTW energy efficiency for the operation with the electric motor of 72% — calculated with the product of the efficiencies of the main electric powertrain components: electric motor efficiency: 90% (Jurca et al., 2015), battery discharge efficiency: 94.5% (Du et al., 2017), battery traction motor efficiency: 88.9% (Du et al., 2017) and transmission efficiency: 95.5% (Du et al., 2017); and a recuperation efficiency for the regenerative braking system of 21% (Perrotta et al., 2012).

Although this simplification excluded the consideration of non-linearities between instantaneous power and actual energy use in a bus, yet the backwards-calculating energy use rate estimation method made it possible to estimate TTW energy use at each data point based on route-specific and time-specific driving cycles data. Thus, this method and real-world bus operation data enabled to use route-specific and time-specific TTW energy use data in the optimisation model instead of the use of constant average values for the operation of buses on bus routes.

Once the model had been solved for the first chunk of data, the SOCs in the batteries of buses were known at the end of the three-minute time interval, and thus, this information could be used in the consecutive chunk of data. The decisions from the optimisation were then considered in the simulations and run. Whether all-electric operation was eventually used or not during a time step in the simulation was depended on the requirement that enough electricity had to be available to drive all-electric over that entire time step. This requirement was applied in all scenarios.

Note: The backwards-calculating energy use rate estimation method was also used to calculate the diesel consumptions of the bus fleets in the BAU and HYB scenarios.

Results
Total TTW energy use, energy savings and all-electric operation of the bus fleet were estimated for each day of the two weeks of bus operation data. The arithmetic mean values are presented as results in the following. The total TTW energy use of the bus fleet is presented as the total TTW energy use in megajoule (MJ\text{TTW}) per kilometre (km). The estimations from the backwards-calculating energy use rate estimation method were validated through comparison to real-world data from Curitiba as well as analysis and review of the functioning of charge-depleting and charge-sustaining operation modes in the simulations (see Paper III for more details).

Energy savings are presented as the percentage (%) of the reduced amount of energy use in the HYB and PLUG scenarios compared to the BAU scenario. All-electric operation is presented as
percentage of total all-electric distance (TAED) to the total operation distance of the bus fleet as well as percentage of total all-electric time (TAET) to the total operation time of the bus fleet.

The simulation found a large potential to save energy with an increasing degree of electrification in the powertrain (Figure 15). The range bars show the data spread between the minimum and maximum values for the bus fleet considering all operation days. Three measures made energy savings possible: 1) All-electric operation using electricity generated from regenerative braking. This technology saved 17% of energy as shown in the HYB scenario. The same technology was also used in the PLUG scenarios. Additionally, the following two additional advances were applied in the PLUG scenarios that saved in total additional 10%-points of energy. 2) Buses employed larger batteries in terms of nominal capacity. The batteries were recharged during operation using opportunity charging. As a result, the all-electric operation could be used more and longer, which saved additional 8%-points of energy. Lastly, 3) Batteries were charged to the initial SOC at operation start considering the possibility of overnight charging in a bus depot. This amount of electricity was used for all-electric operation and gave additional 2%-points of energy savings. Altogether, energy savings of 27% could be achieved in the PLUG scenarios on average.

Only marginal differences between the different management strategies were found concerning energy savings. Obviously, a systematic replacement of conventional bi-articulated buses by either hybrid-electric or plug-in hybrid-electric bi-articulated buses is very effective to achieve energy savings in the operating bus fleet. The marginal differences between the PLUG scenarios further indicate that an operational optimisation through the tested management strategies does not lead to mentionable energy efficiency gains.

Another observation is that scenarios PLUG-A (27.65 MJTTW/km) and PLUG-B (27.67 MJTTW/km) achieve slightly lower levels for total energy use in comparison to the PLUG-C scenario (27.88 MJTTW/km). This is counter-intuitive as the PLUG-C scenario aims to minimise the total energy use and therefore, this scenario should show the least total energy use. The reason for this observation originates from the Greedy algorithm that finds an optimal solution at present without consideration of consequences in the future, i.e. an optimal solution is found for the current time interval without any consideration of the next time intervals. While this leads to several local optimal solution, it does not imply to find a global optimal solution as in the case if all operation data was considered at once and likewise, the model was only solved one time. The expectancy would be that PLUG-C achieves the lowest total energy use. However, this would exclude the possibility to react on the operational uncertainty from the deviation from the ideal timetable due to car accidents, congestions or other unexpected events.

It can be concluded that a systematic change towards more electrification is more effective to save energy than the choice of a management strategy for the plug-in hybrid-electric bi-articulated bus fleet. Although no significant differences between management strategies were found concerning energy savings, the choice is very relevant for maximisation of the total all-electric operation, as presented next.
Management Strategies for an Electrified Bus Fleet

Figure 15: Total energy use and total energy savings of the bus fleet in the scenarios (formatted figure from Paper III)

Figure 16 shows the findings for all scenarios concerning the total all-electric operation measured by TAED and TAET. Only conventional buses are deployed in the BAU scenario and thus, all-electric operation was impossible. The hybrid-electric buses in the HYB scenario drove all-electric for 14% of their total operation distance (TAED result), which corresponds to 20% of their total operation time (TAET result). In the case of the PLUG scenarios a TAED of 40% and TAET of 43% were achieved on average considering all management strategies. However, the choice of a management strategy strongly matters in this respect. The least TAED (17%) and TAET (20%) were achieved by management strategy C. In comparison, management strategies A and B achieved the same result with a TAED of 30% and TAET 36%. Based on this finding, no additional benefit was found from whether to include knowledge about the average energy intensity of buses on a BRT route or not — as done in management strategy B.

The most TAED and TAET could be achieved by applying management strategies that aimed to maximise the all-electric operation. However, management strategy D — Maximise total all-electric time of bus fleet — could maximise both objectives compared to management strategy E. The PLUG-D scenario reached a TAED of 61% and TAET of 64%, whereas management strategy E achieved a TAED of 60% and TAET of 57%. The simultaneous maxima in the PLUG-D scenario, and particularly, the achievement of also maximising TAET is presumably again a result by the Greedy algorithm. In summary, potential gains by 31%-points for the total all-electric distance and 28%-points for the total all-electric time were estimated through the RTO approach using management strategy D instead of the commonly used and simpler management strategy A. Therefore, the choice of a management strategy is very relevant for maximisation of the total all-electric operation in the case of a plug-in hybrid-electric bus fleet.
Recap of chapter 3

This chapter presented a real-time optimisation (RTO) model for the operational optimisation of the charging schedule and/or all-electric operation of a plug-in hybrid-electric bus fleet subject to operational uncertainty. The RTO model used route-specific and time-specific driving cycle data as well as elevation profile data to estimate the Tank-to-Wheel (TTW) energy use of the buses. The RTO model and five management strategies were simulated and evaluated for the hypothetical case of a plug-in hybrid-electric bi-articulated bus fleet in a subsystem of Curitiba’s BRT system — the plug-in hybrid-electric (PLUG) scenarios with management strategies A–E. In addition, the hypothetical case of a hybrid-electric bi-articulated bus fleet was simulated — the hybrid-electric (HYB) scenario. The scenarios were compared to the current situation, in which conventional bi-articulated buses are used — the business-as-usual (BAU) scenario. Simulations and insights are based on two weeks of real-world bus operation data from Curitiba.

The simulations revealed potential energy savings of 17% and 27% in the HYB and PLUG scenarios compared to the BAU scenario, respectively. While the degree of electrification could considerably reduce TTW energy use, no significant differences were found among the management strategies in the PLUG scenarios. This, however, was different concerning the all-electric operation. Depending on the management strategy, a potential of 17–61% for the total all-electric distance was estimated and 21–64% for the total all-electric time of the bus fleet compared to the total operation distance and time, respectively. The PLUG scenario with management strategy D — that aims to maximise the all-electric operation time of the bus fleet — achieved simultaneous maxima for both the total all-electric distance and time. Thus, potential gains by 31%-points for the total all-electric distance and 28%-points for the total all-electric time were estimated through the RTO approach considering management strategy D in comparison to the commonly used and simpler management strategy A: Prioritise buses for charging by arrival times at the charging station (first come, first served).

Overall, a systematic replacement of conventional buses by either hybrid-electric or plug-in hybrid-electric buses is very effective to achieve energy savings. However, only marginal
differences between the different management strategies were found concerning energy savings. In comparison, the choice of a management strategy is very relevant for maximisation of the total all-electric operation in the case of a plug-in hybrid-electric bus fleet. Thus, the implementation of a systematic change from conventional buses to plug-in hybrid-electric buses is recommended in combination with using the RTO approach to manage the charging schedule and all-electric operation.
4 OSEMSYS-PULL FOR MONTE CARLO SIMULATION

This fourth chapter is dedicated to the development of the new software system — OSeMOSYS-PuLP — that makes it possible to run a Monte Carlo simulation with the OSeMOSYS modelling framework in a convenient and automated way. The tool’s applicability is demonstrated by using a case study with real-world bus operation data from Curitiba’s bus transport system. The focus is on the representation of real-world behaviour and associated uncertainties in the area of long-term energy systems modelling. The research presented in this chapter is based on scientific paper IV (referenced as Paper IV).

4.1 OPPORTUNITIES AND THE CHALLENGE

The transformation of an energy system is a cost and time-intensive process that implies potential benefits and drawbacks in the future. Those should be carefully considered and evaluated before a transformation starts. The evaluation process of transformation strategies relies strongly on the development and simulation of long-term energy planning scenarios in the case of energy systems. For their development, modelling frameworks are an indispensable tool due to their cost-efficiency and safety concerning the quantification and evaluation of changes on the economy, environment and/or society (Subramanian et al., 2018).

As earlier mentioned in the literature review, this thesis focuses on the OSeMOSYS (Open Source energy MOdelling SYStem) modelling framework. OSeMOSYS uses an open source bottom-up modelling approach for the development and optimisation of techno-economic long-term energy systems models and planning scenarios (Gardumi et al., 2018; Howells et al., 2011; OSeMOSYS Steering Committee, 2019). OSeMOSYS has been widely used for research to generate insights and understanding about structural changes of energy systems and their associated impacts on economy, environment and society, e.g. see studies by (Leibowicz, 2018; de Moura et al., 2018; Dhakouani et al., 2017; Pinto de Moura et al., 2017; Moksnes et al., 2017; Welsch et al., 2014). Features and capabilities of OSeMOSYS are well-described in the literature, e.g. see the OSeMOSYS’ development papers by (Gardumi et al., 2018; Howells et al., 2011), and therefore, only a brief introduction is given in this thesis.

A modelling process usually starts with the design of a reference energy system (Beller, 1976) that represents the real-world energy system being subject to an analysis. The reference energy system maps the flows of energy sources within the real-world energy system — from the extraction of primary energy sources, over the transport and conversion to secondary and tertiary energy sources, to the transport or transmission to the final energy use by energy-consuming services. The representation of those stages is deterministically designed in OSeMOSYS, i.e. a model instance always generates the same output dataset from the same input dataset. The user of OSeMOSYS provides user-specific data in the input dataset that includes, for example, technology investment options, energy demands, lower and/or upper capacity limits for technologies, renewable energy targets, emissions limits, and so forth. Ultimately, the input dataset defines the requirements from which an instance of the modelling framework is generated. It can be an energy model for a single region or multi-regional model. Linear
optimisation is used in OSeMOSYS, which implies linear relationships between decision variables and equations.

The functional design and structure of OSeMOSYS is divided into seven components (Gardumi et al., 2018; Howells et al., 2011): 1) objective function — an equation for the net present cost (NPC). The NPC states the sum of all costs and revenues in an energy system over the considered time period in an analysis discounted to the first year of the time period. The NPC is minimised to find an optimal techno-economic solution to meet the user-defined requirements at the lowest cost; 2) costs — equations to account capital costs, variable and fixed operating costs, salvage values, and the discount rate; 3) storage — equations to define energy storage technologies; 4) energy balance — equations to balance energy production and consumption; 5) emissions — equations to account emission intensities, limits and penalties; and 6) other constraints — equations to account limits on capacities or productions of technologies.

Some more functionalities have been developed and released for OSeMOSYS as time passed, such as: 1) enhanced storage representation (Andrea et al., 2020); 2) reserve capacity (Welsch et al., 2015); 3) cost of cyclic operation of fossil power plants (Gardumi, 2016); and 4) smart-grids and demand-side flexibility (Welsch et al., 2012). All functional components together aim to create a representative model of an energy system subject to analysis and optimisation.

In addition to a representatively designed modelling framework, a representative model also requires representative input data. The latter should be collected from the real world rather than being based on arbitrary assumptions. Aggregated data such as average values, i.e. mean, median or mode, are commonly used as input data. One advantage of using an average value is the potential representation of large amounts of data in a single value. However, this reduction of complexity has limitations, such as restriction of the dimensionality of an analysis to the aggregation level, presumption of correctness, a potential impossibility to trace back the average value to the original raw data, etc. For example, average values are often used in the demand side of an energy system model, e.g. for the energy intensity of road vehicles. However, heterogeneity and randomness of real-world behaviour are not captured by a single input value. This, in turn, can limit transparency and confidence in insights and conclusions from a model. Although this was a non-exhaustive list of examples, it depicts the demand for enhancements, e.g. in the OSeMOSYS modelling framework, with the goal for a more detailed representation of real-world behaviour in energy systems models.

In contrast to average values, probability distributions can represent more of the heterogeneity and randomness of real-world behaviour. Those can be either parametric or empirical non-parametric distributions. Parametric distributions assume a certain shape for the distribution of data. This shape can be mathematically described using a fixed set of known parameters. In comparison, empirical distributions do not assume any shape and are empirically generated from measurements. The latter usually requires large amounts of data to generate a representative empirical distribution for heterogenous real-world behaviour.

Open data movements have considerably gained in importance for science recently (Pfenninger et al., 2017). In this regard, the evolvement and accessibility of software and computer technologies can assist fast data preparation and analysis processes nowadays (Chen et al., 2015; Jin et al., 2015). One example is Curitiba’s open data online platform (UFPR, 2019), where bus operation data from the city’s public bus transport system is made accessible for free. The data originates from the application of an ITS concept in the city. The operation data of buses is recorded and transmitted to a database where the data is stored. From there, the data can be made available and retrieved for analyses. Such large raw datasets provide new possibilities and
can increase confidence and transparency of modelling insights compared to relying on already aggregated data.

The challenge is to utilise large datasets in energy systems models with the aim to represent real-world behaviour and randomness. Randomness further implies uncertainties. While many studies have already demonstrated the utilisation of large amounts of real-world data, as presented earlier in the literature review chapter, its use in long-term energy systems modelling remains a challenge when demanding certain requirements, such as: 1) in addition to open data, all steps in the modelling process shall be open source, which starts at the modelling framework; goes to the programming language; and to the solver that determines an optimal solution; and 2) the simulation process shall be run in a convenient and automated way. The first requirement is fulfilled by the OSeMOSYS modelling framework. To extend OSeMOSYS’s functionality and to meet the second requirement, a new code implementation was developed and embedded into a wider software system with the purpose to make a Monte Carlo simulation possible in a convenient and automated way — OSeMOSYS-PuLP. A Monte Carlo simulation can be used to quantify and evaluate the impact of exogenous uncertainties in the input dataset on insights and conclusions. Eventually, this feature overcomes the limitation of OSeMOSYS that uncertainty, due to randomness in the real world, has not been represented so far, since it is a deterministic modelling framework.

4.2 SOFTWARE SYSTEM OSEMSYS-PULP

OSeMOSYS-PuLP is a software system for empirical deterministic-stochastic modelling and optimisation. The name is compound of OSeMOSYS and PuLP. The latter stands for the Python software package PuLP: A Linear Programming Toolkit for Python (Mitchell et al., 2011). Python is a popular open source programming language (Python Software Foundation, 2019, p.6). OSeMOSYS-PuLP facilitates the use of real-world datasets (which is the empirical component) in a long-term energy system model that is based on the OSeMOSYS modelling framework (which is the deterministic component) and enables the possibility of a Monte Carlo simulation (which is the stochastic component) in a convenient and automated way.

OSeMOSYS-PuLP was coded and tested in Python 3.6.6 (Python Software Foundation, 2019, p.6) using the Python packages PuLP for linear optimisation modelling (Mitchell et al., 2011); Pandas for data handling (McKinney, 2010); NumPy for importing probability distributions (Oliphant, 2006); and Xldr for generating and reading of spreadsheet files (Machin and Lingfo Pty Ltd, 2019). Moreover, the COIN-OR Branch-and-Cut MIP (CBC) solver (johnjforrest et al., 2019, p.3) is used by default to solve the optimisation model. This solver is an open source mixed-integer programming (MIP) solver and the default solver in the python package PuLP. Besides, other common solvers are supported and listed online, e.g. see (Mitchell et al., 2019).

While other code implementations of the OSeMOSYS modelling framework have been already existing for years, e.g. coded in GNU MathProg (GNU MathProg, 2015), GAMS (GAMS Software GmbH, 2019) and Python-Pyomo (Hart et al., 2017; Hart et al., 2011), OSeMOSYS-PuLP has some distinct differences and extensions:

1. The feature of a Monte Carlo simulation is a substantial addition to the use of the OSeMOSYS modelling framework. This makes it possible to quantify and evaluate the impact of exogenous uncertainty on insights and conclusions.

2. The input data file is a spreadsheet file, which makes it possible to use a spreadsheet software as graphical user interface. This facilitates data provision and review processes
The output data file is a spreadsheet file, too, which stores the optimal values for each variable and its index set on separate tabs. This supports a rapid review of the output data and further post-analysis.

The user can select specific results that should be saved in the output file. This is advantageous if only a few variables are of interest, and by excluding other variables from the writing to the output file, the run-time can be reduced.

The model representation is form of a concrete model, whereas other code implementations of the OSeMOSYS modelling framework use abstract models. Concrete models are more intuitive as all decision variables, parameters, constraints and index sets are explicitly shown in the code. This facilitates the understanding of the logic in the model. A syntax comparison of the different code implementations is provided in Figure 17. In comparison, abstract models use placeholders for decision variables, parameters, constraints and index sets. When the input data is loaded, an instance of the abstract model is initialised, and the concrete model is built then. Overall, the code of OSeMOSYS-PuLP is less verbose than, for example, Python-Pyomo. Furthermore, code readability is crucial for communication and comprehension of the equation system’s logic. Moreover, this advantage is noteworthy as the OSeMOSYS modelling framework is used as a teaching tool to a wide audience (OpTIMUS, 2019). Additionally, the concrete modelling approach provides an advantage for running a Monte Carlo simulation. The concrete modelling approach enables to use Python specific functions during the construction process of the linear equation system, e.g. use of probability distribution functions from NumPy. The reason for this is that decision variables, parameters and constraints are initialised as these are constructed. This enables to only overwrite those values of some parameters that shall be considered in a Monte Carlo simulation rather than loading all data and reconstructing the whole model and its parameters from scratch. In comparison, in the case of abstract models, the whole model is initialised and constructed when the input dataset is loaded. This, however, prevents any possibility to use Python specific functions during the construction process. As a result, any assignment of new values to specific parameters is impossible and hence, in the case of a Monte Carlo simulation, the whole input dataset and model would be needed to be reloaded and reconstructed from scratch, respectively.

Plenty of possibilities exist to contribute and develop OSeMOSYS-PuLP further due to its concrete modelling approach and syntax as well as flexibility and open source design. Examples for future development could be some pre- and post-processing of the input dataset and output dataset, respectively, e.g. as done in the case of developing otool OSeMOSYS tools for energy work by (Usher, 2019) — a recently released Python package to facilitate typical pre- and post-processing work for the use of OSeMOSYS.
4.3 MONTE CARLO SIMULATION OF UTOPIA

The demonstration and validation of OSeMOSYS-PuLP was done by using an earlier application example of the OSeMOSYS modelling framework from its introductory paper in 2011 (Howells et al., 2011) — the model of Utopia. Some updates to the dataset have been made since then and therefore, the latest published dataset was used — the BASE: Utopia Base Model dataset (KTH-dESA, 2017, p.). By using Utopia as proof-of-concept case study, the dimensions of the model and analysis were kept the same as in the application example of the original OSeMOSYS code implementation in GNU MathProg. This facilitates a straight-forward comparison of the results obtained from OSeMOSYS-PuLP to the GNU MathProg version. The research process is summarised in Figure 18 and described in the following.

The reference energy system of Utopia represents a single region that is not explicitly further defined in any geographical dimension. Figure 19 shows the reference energy system consisting of energy carries (illustrated as lines) and technologies (illustrated as white blocks) that both aim to provide energy to energy services (illustrated as the white blocks on the right side in Figure 19).
Three energy services exist in Utopia: 1) lighting, 2) heating, and 3) passenger transport. Lighting and heating demands depend on the daytime and season, respectively. The lighting demand is higher during the night, and the heating demand is higher during the winter. While only one technology is available to meet the lighting service, namely lightbulbs (RL1), the heating service can be provided by either electrical heating (RHE) or oil heating (RHO). Passenger transport can be met by three different transport technologies, which include electric vehicles (TXE), diesel vehicles (TXD) or petrol vehicles (TXG). Thus, electricity, diesel and petrol are the final energy sources for the transport sector in Utopia. Five technologies are available to generate electricity: coal (E01), nuclear (E21), hydro (E31), pumped-storage (E51) and diesel (E70). While hydro and pumped-storage are endogenous energy sources, the remaining energy sources must be imported. For example, diesel (DSL) and petrol (GSL) are imported through import technologies IMPDSL1 and IMPGSL1, respectively, as well as can be produced from imported crude oil (IMPOIL1) in an oil refinery (SRE). Lastly, coal and uranium are imported, too, but through import technologies IMPHCO1 and IMPURN1, respectively.

The white blocks in Utopia’s reference energy system require input data and thus, those represent entry points for the use of real-world data. Obviously, real-world data is of interest at all stage in the reference energy system concerning the flows of energy sources between technologies and services. In this case study, the energy service of passenger transport was selected as an example to demonstrate OSeMOSYS-PuLP’s capabilities.
The energy demand for transport is given by the parameter *Accumulated annual demand* in the OSeMOSYS modelling framework. The *Accumulated annual demand* defines the total annual final energy use by all transport-related end-users in Utopia and is separately provided for each modelled year in the input dataset. The data is inserted on a yearly basis from 1990 to 2010, i.e. one fixed value for each modelled year as common for deterministic modelling framework.

To model more heterogeneity and randomness as in the real world, the input value for the *Accumulated annual demand* would be needed to change in each simulation of the model. If the model should be run one hundred times, one hundred datasets would be needed in any of OSeMOSYS code implementation that have existed so far, i.e. GNU MathProg, GAMS, Python-Pyomo. This is quite inconvenient as separate dataset files are required for each run. OSeMOSYS-PuLP overcomes this inconvenience and makes it possible to run the model in a convenient and automated way.

A probability distribution is needed as input data so that OSeMOSYS-PuLP can draw random values from it and uses each of those for the parameter *Accumulated annual demand* in each simulation. One way to create a probability distribution is the analysis of a large real-world dataset to generate an empirical probability distribution. As Utopia is not further declared than as a generic region, it is assumed to be a city in this proof-of-concept case study. As earlier mentioned, Curitiba’s open data online platform is an available and free resource for public bus transport data (UFPR, 2019), and the operation data from the city’s public buses was used in this case study. This also provides an examples to Curitiba on the possibilities how to use its open data and the integration into long-term systems planning.

Curitiba’s passenger transport system consists of many transport modes, such as public buses, cabs, private cars, but no metro system. Only public buses were considered due to data availability as well as to analyse more distinctly its importance in a long-term energy system model. Overall, the dimensions and input dataset are the same as in the original introduction paper of the OSeMOSYS modelling framework, but the input data for the parameter *Accumulated annual demand* is based on the real-world bus operation data from the entire public bus transport system in Curitiba, i.e. all bus routes — regular and BRT routes. The bus
operations data originates from all buses operated during the period of 30 January 2017 to 15 July 2018, i.e. 1.5 years.

The data preparation included data cleaning for incomplete data points as well as exclusion of outliers. Some additional calculations were needed as the dataset only contained recorded data for the bus identification number, GPS coordinates and timestamp in each data point. However, the TTW energy use of each bus for each data point was needed and thus, the speed, longitudinal acceleration and road gradient were calculated for each data point. A full description of the data preparation process is provided in the supplementary material of Paper IV. Once those quantities were estimated, the driving cycle and elevation profile could be built. Both were needed to estimate the TTW energy use of the buses. While ADVISOR was used to estimate the energy use of buses in Paper I and Paper II, the tool was unsuitable in this study due to the much larger amount of data. Hence, instead of running thousands of simulation in ADVISOR, a TTW energy use prediction model was developed based on the theory of the backwards-calculating energy use rate estimation method as earlier described and in Paper III. The prediction model is similar as the one in Paper III, but more advanced to account more of the potential non-linearities in the powertrain of a bus. The full description and validation are provided in the supplementary material of Paper IV.

Briefly summarised: Multiple linear regression was used to derive a prediction model for the TTW energy use based on the theory of the previously used backwards-calculating energy use rate method. The model was fitted using TTW energy use data obtained from simulations of a conventional bus model in ADVISOR. The advantage of applying the prediction model was a fast calculation for all TTW energy values for all data points in the 1.5 years of bus operation dataset. Moreover, this data provides more detailed insights into TTW energy use variations in the bus fleet and complements the aggregated average values that are published online by Curitiba’s public transport authority URBS (URBS, 2018a).

The value for the input parameter *Accumulated annual demand* was calculated by using the three TTW energy use values representing operations on Weekdays, Saturdays and Sundays, and multiplying those with the respective number of kilometres driven by the bus fleet over the duration of one year. Since the bus operation data contained data for 1.5 years of operation, bootstrapping could be used generate a set of random values for the annual energy use of the bus fleet. The results are provided in Table 8.

Eventually, this set of random values was used to create an empirical distribution of values for the *Accumulated annual demand*. The values of this empirical distribution were normalised to the yearly values in the Utopia dataset for the *Accumulated annual demand* over the period 1990–2010. This gave separate empirical distributions for each modelled year as shown in Figure 20. Besides, by using normalisation, the dimensions were kept the same as in the Utopia analysis of the OSeMOSYS introductory paper by (Howells et al., 2011).

| Table 8: Descriptive statistics of the annual energy use values (TJ/year) in the dataset obtained from bootstrapping (Paper IV) |
|---|---|---|---|---|---|---|---|---|---|
| N (-) | Mean | S.D. | Min. | Q25 | Median | Q75 | Max. | Skew. (-) | Kurt. (-) |
| 100 | 1608.62 | 1.31 | 1605.82 | 1607.66 | 1608.60 | 1609.47 | 1611.46 | 0.011 | -0.616 |
Lastly, one additional constraint was added that demands to keep Utopia’s CO₂ emissions below a certain threshold. The threshold amounts to 163.5 tonnes of CO₂ over the period 1990–2010 and was obtained from solving one time the Utopia model using the default dataset **BASE: Utopia Base Model**. This constraint implies that CO₂ emissions in Utopia must be stabilised at least, which is an analogous to the real world concerning the climate target nowadays.

**Results**

OSeMOSYS-PuLP was run one time with the default Utopia dataset and determined an optimal value for the net present cost (NPC) for Utopia over the period 1990 to 2010 of 29 446.9 M$ (million US dollar). This is the same value that is found by the GNU MathProg code implementation of the OSeMOSYS modelling framework. Thus, OSeMOSYS-PuLP was validated. The first simulation is referred to as reference case for comparisons to the Monte Carlo simulation, in which the model was run 100 times with a random variation of the parameter Accumulated annual demand for the passenger transport. The output data from the first simulation is further assumed to be the most likely scenario, as it was used to normalise the empirical distributions for the Accumulated annual demand, around which the other values are either lower or higher.

The cumulative distributions of absolute changes for NPC, CO₂ emissions (CO₂), electricity consumption (ELC) and diesel consumption (DSL) in Utopia over the period 1990–2010 are shown in Figure 21. The results verify the observance of the CO₂ limit that must not be exceeded further than the determined value as in the reference case (Figure 21a). Above the reference case, i.e. where the Accumulated annual demand of passenger transport is larger than in the
reference case, electricity (ELC) is used as a transport fuel (Figure 21b). Due to its carbon neutrality according to the input dataset, no more CO$_2$ emissions are released and rather stabilise the amount of CO$_2$ at the level in the reference case (Figure 21a). However, the electric transport technology (TXE) has got higher capital cost and fixed cost than diesel transport technology (TXD). Consequently, the NPC increases (Figure 21c). Besides, since the CO$_2$ emissions limit must be satisfied, no additional capacity is built for diesel transport technology (TXD) and likewise, the diesel consumption (DSL) remains at a constant level (Figure 21c).

In comparison, below the reference case, i.e. where the Accumulated annual demand of passenger transport is smaller than in the reference case, the diesel consumption is reduced and likewise, CO$_2$ emissions (Figure 21d). An obvious correlation can be observed between diesel consumption (DSL) and CO$_2$ emissions (CO2) in this regard (Figure 21d). Since less diesel is consumed, less of the diesel import technology (IMPDSL1) needs to be built. Consequently, the NPC decreases (Figure 21c).

In summary, the electric transport technology (TXE) and electricity (ELC) are used in all cases in which more Accumulated annual demand is demanded than in the reference case (Figure 21e), whereas the diesel transport technology (TXD) and diesel (DSL) are used in the opposite cases (Figure 21e). Accordingly, CO$_2$ emissions either stabilise or decrease, respectively (Figure 21f).

The petrol transport technology (TXG) was not used in any of optimal solutions despite its lower fixed cost (48 M$/GW) compared to the diesel transport technology (TXD) (52 M$/GW). However, its variable cost is higher than for diesel (DSL), namely the petrol import technology (IMPDSL1, 15 M$/PJ) compared to the diesel import technology (IMPDSL1, 10 M$/PJ). The remaining cost parameters are the same for both technologies as well as have the same emission activity ratio. Besides, petrol (TXG) is not a competitive techno-economic option against the electric transport technology (TXE) concerning both NPC and CO$_2$ emissions.

In addition to understanding how the Accumulated annual demand influences the energy demand and supply in Utopia, the probability was quantified for the outcomes. This can be done for every parameter. The NPC is used as an example in the following due to its overall importance by being the objective function in OSeMOYS. The probability distribution for the NPC is shown in Figure 22. Value intervals are used for the absolute changes of the NPC and sorted into a histogram.

One insight is, for example, that a change of the NPC within a range of ±4 M$ around the reference case will happen with a probability of 60% (i.e. 13%+17%+17%+13%). Moreover, NPCs of more than 8 M$ are unlikely considering the associated probability of only 6%. This is important to know as the NPC value trend increases non-linearly above 8 M$. This concerns those few cases that possess a much higher Accumulated annual demand due to exogenous uncertainty introduced by considering the real-world behaviour from Curitiba’s bus transport system in Utopia’s passenger transport sector.
Figure 21: Cumulative distributions of absolute changes for net present cost (NPC), CO₂ emissions (CO₂), electricity consumption (ELC) and diesel consumption (DSL) in Utopia from 1990 to 2010 based on the output data from the reference case and the Monte Carlo simulation. The horizontal axis shows the cumulative distribution ranging from 0% to 100% (formatted figure from Paper IV)

A short remark regarding the rather evenly distributed values of the Accumulated annual demand by each modelled year as earlier shown in Figure 20: Despite the rather evenly distributed empirical distributions, they still represent a data-driven decision-making approach based on real-world data. They further caused structural changes in Utopia’s energy system considering the quantified exogenous uncertainty of the parameter Accumulated annual demand. The new insight generation capabilities of OSeMOSYS-PuLP were demonstrated when using a Monte Carlo simulation within the OSeMOSYS modelling framework. While one parameter was chosen in this study, more parameters could be included in the future. In addition, other types of probability distributions could be used. Certainly, the complexity in an analysis can be increased. Nevertheless, in this proof-of-concept case study, the Monte Carlo simulation capabilities of OSeMOSYS-PuLP were demonstrated, and new data-driven insights generated.
The new feature of a Monte Carlo simulation for the OSeMOSYS modelling framework provides new possibilities for data-driven decision-making considering exogenous uncertainties. A Monte Carlo simulation can be applied to parameters that are associated with uncertainty, such as the energy demand in the transport sector. While a single value for an input parameter leaves out information about probability of certain outcomes, the use of a probability distribution complements those information. The result is a distribution of possible outcomes accompanied with a probability statement for each outcome. e.g. as the NPC distribution in the case of Utopia due to uncertainty in the Accumulated annual demand. This expands the set of information and enables decision makers to understand deeper possible outcomes for expected cost and revenues in the transformation of an energy system, i.e. the information supports decision makers by assessing uncertainties and including the gained insights into the decision-making process. Eventually, this shall prevent any unexpected event in the future based on the analysis of information that is available at present. Moreover, the open data from Curitiba made it possible to model and represent more detailed the transport system in a long-term energy system model. This demonstrated the efforts and value generation made by the city through collecting, storing and making the public bus operation data available to the research community.

Recap of chapter 4

This chapter presented the new software system OSeMOSYS-PuLP that extends the functionality of the OSeMOSYS modelling framework by the feature of a Monte Carlo simulation. The benefits of OSeMOSYS-PuLP are 1) Monte Carlo simulation for stochastic optimisation; 2) the input data file is a spreadsheet file; 3) the output data file is a spreadsheet file; 4) the model user can select specific results that should be saved in the output file; 5) the model representation in form of a concrete model, which facilitates code readability and logic comprehension; and 6) the syntax, flexibility and open source design offer many possibilities for development in the future.

In addition, a proof-of-concept case study was presented based on the Utopia dataset that was complemented by real-world bus operation data from Curitiba. OSeMOSYS-PuLP was validated by comparing the output data to the results from the original code implementation in GNU MathProg. A Monte Carlo simulation was run to analyse the influence of exogenous uncertainties. The simulation found that this uncertainty caused structural changes in Utopia. Moreover, probabilities for the deviation from the expected NPC were estimated. Overall, a more advanced analysis of the Utopia case was possible, including an assessment of impacts from capturing the randomness and heterogeneity of the real world, on insights and conclusions.
5 CONCLUSIONS

This fifth and concluding chapter states the key messages from the research and findings concerning the thesis’ objective and research questions. Contributions to the scientific literature are summarised. Moreover, limitations are described and recommendations for future work are given. Lastly, the impact of the research is described.

5.1 KEY MESSAGES

The research in this doctoral thesis showed that transition technologies, such as advanced buses, models and planning tools, can contribute and support the transition phase of bus transport systems towards the introduction and an effective use of electricity as a vector for decarbonisation. In the view of the fact that global warming poses a threat to the earth and humankind, the necessity for reducing GHG emissions becomes comprehensible.

In this respect, the overall contribution of this thesis is that its research findings, applied methods and developed tools can be used to support and inform analysts and decision-makers in the area of transport and energy systems planning in their decision-making process to develop and assess different technological options and strategies at different levels while considering associated uncertainties:

- Bus technology level: The thesis provides insights and methodological approaches to compare different types of buses concerning energy use, emissions, costs, influential factors and operational uncertainty.
- Bus fleet management level: The thesis provides a real-time optimisation model to manage a plug-in hybrid-electric bus fleet according to different management strategies considering operational uncertainty.
- Long-term system planning level: The thesis provides a software system — OSeMOSYS-PuLP — to make strategic techno-economic decisions considering exogenous uncertainty.

The C40-city of Curitiba was used as a case study in this thesis, yet, applied methods, insights and key messages are also valuable and potentially applicable to other C40 and non-C40 cities globally. The key messages derived from the research findings are mapped below to the respective research questions in thesis from Section 1.4:

1. How much can energy use, GHG emissions and cost of transport service be reduced by advanced buses?

Considerable potentials were estimated to reduce energy use in the operation phase of buses when operating advanced (electrified) buses instead of conventional buses. For example, energy savings of 30% and 58% were found if hybrid-electric and plug-in hybrid-electric two-axle buses replace the conventional two-axle bus in Curitiba, respectively. Furthermore, energy savings in the operation also imply avoidance of energy expended and emissions released to produce and supply fuels. The combined reductions amount to 75% of fossil energy savings and 72% of GHG emissions reductions on the Well-to-Wheel (WTW) scope when using a plug-in hybrid-electric two-axle bus instead of a conventional two-axle bus. The percentages correspond to an absolute
reduction of 1.1 kgCO₂e for every kilometre driven, which highlights the large potential when using electrification for decarbonisation in the case of Curitiba.

In addition to an electrified powertrain, the utilisation of the passenger carrying capacity in a bus is important to effectively transport passengers in terms of energy use per passenger-kilometre in the operation phase. The analysis of a conventional bi-articulated bus showed that this bus can be more energy-efficient than hybrid-electric two-axles buses in terms of energy use per passenger-kilometre. Nevertheless, the combination of an electrified powertrain and large passenger carrying capacity as in the case of a hybrid-electric articulated bus, or a higher degree of electrification despite a smaller passenger carrying capacities as in the case of the plug-in hybrid-electric two-axle bus, can both achieve further reductions concerning energy use and emissions.

The analyses also revealed that an absolute change of energy use to a passenger load change decreases with increasing degree of electrification in a bus, i.e. conventional buses are impacted the most by passenger load changes, followed by hybrid-electric buses and the least for plug-in hybrid-electric buses when operating in charge-depleting mode. Moreover, uncertainties due to varying driving cycles and/or fluctuating fuel prices impact again the most the fuel cost of conventional bi-articulated bus due to its considerable energy use, whereas electrified buses are less influenced. Overall, advanced (electrified) buses can also reduce operational uncertainty concerning an absolute variation of energy use and fuel cost in the operation phase.

Scenarios, in which conventional bi-articulated buses were replaced by more advanced but smaller buses, showed that the operation of those smaller buses can decrease the waiting time from 11 minutes down to 4 minutes for passenger. However, this, in turn, increased the weekly cost of transport service by 30% up to 139%, in the case of one BRT route in Curitiba.

Overall, the research findings showed, from the analyses at the bus technology level, that electrified buses can considerably support the decarbonisation of a bus transport system by using electricity instead of petroleum diesel or more specifically, the biodiesel blend B7. All buses in this thesis used less than 0.5 MJ\textsubscript{TRW}/pkm on average, which is the suggestion by the IPCC to achieve a concentration of 450 ppm of CO₂e in the atmosphere concerning the climate target to limit global warming to 2°C (Creutzig et al., 2015; Edelhofer et al., 2014). Although conventional buses could also meet this requirement, it should be noted that much lower energy use per passenger-kilometre could be achieved by the hybrid-electric articulated bus and plug-in hybrid-electric two-axle bus. Hence, buses that can use electricity to drive should be used to reduce energy use and GHG emissions from public bus transport systems. The higher the degree of electrification and the more electricity is used instead of fossil fuels, the more effective are those transition technologies to decarbonise public bus transport systems already today without relying completely on charging infrastructure.

The C40 network consists of 94 cities in which over 650 million people live (C40, 2019c). Thus, a tremendous advance could be already achieved if all cities were required to introduce transition technologies, such as hybrid-electric and/or plug-in hybrid-electric buses, globally. The joint effort of a structural change could be of high importance to reduce global warming and mitigate the potential severe consequences.

2. What potential exists for energy savings and all-electric operation from the operational optimisation of a plug-in hybrid-electric bus fleet?

A real-time optimisation model was developed, and its concept was tested for the operational optimisation of the charging schedule and/or all-electric operation of a plug-in hybrid-electric bus
fleet subject to operational uncertainty. Moreover, management strategies were simulated and evaluated for the hypothetical case of a plug-in hybrid-electric bi-articulated bus fleet operated in a subsystem of Curitiba's BRT system — the plug-in hybrid-electric (PLUG) scenarios with management strategies A–E. In addition, the hypothetical case of a hybrid-electric bi-articulated bus fleet was simulated — the hybrid-electric (HYB) scenario. Those scenarios were compared to the current situation, in which mainly conventional bi-articulated buses are used — the business-as-usual (BAU) scenario.

The simulations revealed potential energy savings of 17% and 27% in the HYB and PLUG scenarios compared to the BAU scenario, respectively. While the degree of electrification could considerably reduce energy use during operation, no significant differences were found among the management strategies in the PLUG scenarios. This, however, was different concerning all-electric operation. Depending on the management strategy, a potential of 17–61% for the total all-electric distance was estimated and 21–61% for the total all-electric time compared to the total operation distance and time, respectively. The PLUG scenario with management strategy D — that aims to maximise the all-electric operation time of the bus fleet — achieved simultaneous maxima for both TAED and TAET. Thus, potential gains by 28%-points for the total all-electric time and 31%-points for the total all-electric distance were estimated through the real-time optimisation approach considering management strategy D instead of the commonly used and simpler management strategy A: *Prioritise buses for charging by arrival times at the charging station (first come, first served)*.

The methodological framework of the real-time optimisation approach is applicable to any scale of bus transport system using plug-in hybrid-electric buses and opportunity charging. This transferability and flexibility can potentially also improve other less-than-ideal designed bus transport systems in C40 and non-C40 cities globally. Thus, the framework represents a type of *retrofit-solution* to reveal and potentially exhaust more of the available energetic and environmental reduction potentials in non-optimally designed bus transport systems. Moreover, the simulations used real-world bus operation data, i.e. route-specific and time-specific driving cycles and elevation profiles, to estimate energy use in the operation phase instead of the use of average values for the energy intensity of buses or idealised timetables — the latter two represent common simplifications in studies. Only through the integration of real-world bus operation data into the energy use rate estimation method and eventually, into the real-time optimisation model, state-of-charge estimations were possible for each bus in the simulations. Furthermore, based on that data, the management strategies could be tested, and potentials could be estimated. Without this feature, an optimisation of the all-electric operation would have been impossible or would have required additional data. However, additional data such as energy use rate data or state-of-charge data was not available at the time of this research. Thus, the integration of real-world bus operation data should be strived for to develop more advanced models that represent more of the real-world complexity in studies. Eventually, this can possibly generate deeper and more case-specific insights.

Overall, the research findings showed, from the analyses at the bus fleet management level, that a systematic replacement of conventional bi-articulated buses by either hybrid-electric or plug-in hybrid-electric bi-articulated buses is very effective to achieve energy savings. However, only marginal differences between the different management strategies were found concerning energy savings. In comparison, the choice of a management strategy is very relevant for maximisation of the total all-electric operation in the case of a plug-in hybrid-electric bus fleet. Thus, the implementation of a systematic change from conventional buses to plug-in hybrid-electric buses is recommended in combination with using the real-time optimisation approach to
manage the charging schedule and all-electric operation to maximise the total all-electric operation of the bus fleet.

These insights are also relevant considering the climate target and commitments, for example, those made within the C40 network. While the introduction of clean buses as "low and ultimately zero emission buses" according to the C40 Cities Clean Bus Declaration of Intent (C40, 2015b) can achieve decarbonisation through the use of electricity instead of fossil fuels, the gain can be potentially further increased through operational optimisation concerning the charging schedule and all-electric operation of plug-in hybrid-electric buses. Hence, in addition to technological replacements in bus fleets from conventional buses to electrified buses, initiatives and commitments should also include the introduction of operational optimisation to use electricity in the most effective way considering its potential for decarbonisation.

3. How can the influence of real-world uncertainty be represented in and quantified with the long-term energy system modelling framework OSeMOSYS?

The integration of real-world randomness and its heterogeneity in long-term energy systems modelling was achieved by first developing a new code implementation of the OSeMOSYS modelling framework, and then, embedding the code into a wider software system. The new software system is called OSeMOSYS-PuLP and enables to run a Monte Carlo simulation in a convenient and automated way. The functionality of using stochastics is a substantial extension to the application scope of the OSeMOSYS modelling framework.

The proof-of-concept case study demonstrated how real-world bus operation data from Curitiba can be used in long-term energy systems model with the aid of a prediction model based on ADVISOR simulations. From those, an empirical probability distribution was generated and used in OSeMOSYS-PuLP. This methodological framework for empirical deterministic-stochastic modelling is transferable to many other cases and makes it possible for researchers and analysts to generate new sets of conclusions together with associated probability distributions based on the OSeMOSYS modelling framework and real-world datasets.

Overall, the research findings showed, from the analyses at the long-term system planning level, that the Monte Carlo simulation extension in OSeMOSYS-PuLP provides the possibility to assess and quantify the potential impact and probability of exogenous uncertainties on long-term energy planning scenarios. Furthermore, transparency is enhanced and consequently, the reproducibility of studies facilitated by starting the data preparation at the raw data. Ultimately, the transparency shall enable auditing of energy systems modelling studies. This is crucial when considering that such studies can result in spending trillions of US dollars of both private and public funds in the transformation process of transport and energy systems. In this respect, the aspect of openness shall include open raw data sources, an open source modelling framework, an open input dataset, an open source programming language and an open source solver for optimisation models. All these aspects of openness were applied in the proof-of-concept case study in this thesis and are recommended to be also applied in other studies to increase transparency and trustworthiness. Altogether will make it possible to create more case-specific models of transport and energy systems. This enhances understanding to support data-driven decision-making in the planning phase of a transformation based on case-specific real-world data.

The potential for further advancements of transport and energy systems models is given considering open data movements, computational software and hardware evolvements and the opportunities to integrate raw datasets and technologies in reference energy systems in studies (as earlier highlighted by the white blocks representing technologies in Figure 19).
In regard to the C40 network — a data-driven organisation (C40, 2015a) — OSeMOSYS-PuLP could be used to create models of cities or regions based on their own generated data, e.g. available online at (C40, 2019b). The tool would make it possible for analysts to create specific projections and make assessments of plans, targets and commitments, such as the C40 Cities Clean Bus Declaration of Intent (C40, 2015b). This provides deeper insights and estimations that can be used to assess the contributions and effectiveness of C40 cities as well as non-C40 cities concerning the climate target globally.

Overall, initiatives, as for example those in the scope of the C40 network, enhance sustainability in urban transport systems through improved energy efficiency due to electrification of transport systems and reduction of both local and global air pollution, and hereby, contribute to the SDGs by the United Nations (UN, 2018).

**Summary of contributions**

The specific contributions of this doctoral thesis are categorised in the following by analytical advances, methodological advances, and new data and insights:

**Analytical advances**

- Comparative analysis of Tank-to-Wheel (TTW) energy use, Well-to-Wheel (WTW) fossil energy use and WTW GHG emissions of different types of buses in terms of powertrain and chassis, and analysis of influential factors such as: BRT route, operation time, passenger load, driving cycles and fuel prices on TTW energy use and/or fuel cost.
- Real-time optimisation of an operating plug-in hybrid-electric bus fleet subject to operational uncertainty to measure potentials for energy savings and all-electric operation according to five management strategies.
- Use of route-specific and time-specific driving cycles and elevation profiles in the real-time optimisation model to estimate TTW energy use instead of the use of average values for the energy use of buses or idealised timetables.

**Methodological advances**

- Development of a real-time optimisation model and testing of management strategies for the operational optimisation of a plug-in hybrid-electric bus fleet. The model and strategies are scalable and transferable to any bus transport system using plug-in hybrid-electric buses and opportunity charging.
- Development of OSeMOSYS-PuLP for empirical deterministic-stochastic modelling based on the OSeMOSYS modelling framework, which enables the use of a Monte Carlo simulation in a convenient and automated way. This feature is a substantial extension and makes it possible to quantify the potential impact of exogenous uncertainty on insights and conclusions considering associated probability distributions.

**New data and insights**

- New data from TTW energy use, WTW fossil energy use, WTW GHG emissions and fuel cost estimations for conventional bi-articulated buses in comparison with other types of buses in terms of powertrain and chassis.
- New data from the comparison of different bus technology deployment scenarios including conventional, hybrid-electric and plug-in hybrid-electric powertrains in the
case of a bi-articulated bus fleet concerning potentials for energy savings and all-electric operation according to five management strategies.

- New insights from a Monte Carlo simulation using OSeMOSYS-PuLP that rather small exogenous uncertainties in an input dataset, based on real-world behaviour, can potentially have a large impact on structural changes in long-term energy planning scenarios.

5.2 LIMITATIONS AND RECOMMENDATIONS FOR FUTURE WORK

The research used the case study approach to generate empirical-rich and case-specific knowledge and insights for the transition phase of bus transport systems. The case of Curitiba complements other case studies in the scientific literature and hereby, they contribute to a joint generalisation of findings. Some recommendations for future work can be given based on the research of this thesis.

The literature is still quite limited concerning the energetic, environmental and economic analysis of bi-articulated buses and their comparison to other types of buses. While Paper I, Paper II and Paper III made contributions to the scientific literature in this regard, more case studies would provide a broader understanding of potential opportunities and drawbacks globally. Considering that the BRT concept has been increasingly implemented since the year 2000 (BRTdata, 2018a; Hidalgo and Gutiérrez, 2013), more research would be desirable.

The simulations using the real-time optimisation approach estimated potentials for energy savings and all-electric operation for a plug-in hybrid-electric bus fleet. For the application in the real world more data collection and analysis about routes-specific, time-specific and potentially also bus-driver-specific energy use would be needed for a more advanced prediction of the energy use rate and based on that, the state-of-charge in the battery in a bus. As those are input parameters in the real-time optimisation model, comprehensive knowledge is crucial for accurate predictions and an effective implementation of management strategies. In this regard, big data technologies could contribute to store and analyse the tremendous amounts of information that an intelligent bus transport system can generated daily. Case studies that present real-world proof-of-concept projects using big data technologies would be desirable to test the developed framework in action. Moreover, optimal strategies should be further investigated considering jointly bus fleet compositions, ridership variations, driving cycles and other case-specific influential factors.

OSeMOSYS-PuLP can be used create more advanced models and to run a Monte Carlo simulation. Utopia was considered as proof-of-concept case study in this thesis. The next step should be an application of OSeMOSYS-PuLP to a real case. Since this will require large an amount of data to generate probability distributions, a vision could be to build up an automated data collection and processing infrastructure. This could make it possible to represent real-world behaviour at each stage in a reference energy system of an actual energy system. Such a data infrastructure shall automatically generate and periodically update the input dataset. The result could be a model that can represent more of the real-world heterogeneity at each stage and could be also always up to date. Consequently, an analysis could be (automatically) re-run once more recent data is available. Overall, this thesis provides many pillars on which other research can build upon in the future.
5.3 Impact

Paper I, Paper II and partly Paper III were developed in the scope of the research project Smart City Concepts in Curitiba — innovation for sustainable mobility and energy efficiency funded by VINNOVA (Governmental Agency for Innovation Systems) in Sweden. The results contributed to the interdisciplinary project with the goal to identify sustainable technological solutions for urban infrastructure. The research project and findings got lots of exposure through presentations to the former president of Brazil, mayor of Curitiba, city hall of Curitiba, the public transport authority in Curitiba, academia as well as industrial and consulting companies in Sweden and Brazil. The findings of Paper I and Paper II were also presented at two scientific conferences — at IIASA (International Institute for Applied Systems Analysis) in Laxenburg, Austria and in Shanghai, China. The research findings of Paper III have the potential to retrofit existing bus transport systems that operate plug-in hybrid-electric buses and apply opportunity charging. Paper IV contributes to further development of the OSeMOSYS modelling framework as well as supports the OpTIMUS community in its mission “to promote quantitative analysis to inform sustainable development policy” (OpTIMUS, 2019). Measurable impact is shown by some first citations of the scientific papers as well as activities by the energy modelling community on the OSeMOSYS-PuLP GitHub repository available at: (Dreier, 2019). The analytical and methodological advances as well as new data and insights can potentially have an influence on systems modelling and design in the areas of transport and energy systems concerning the development of more complex and detailed models, as well as more optimised systems in the real world.
APPENDIX

Abbreviations and units

ADVISOR  Advanced Vehicle Simulator
Ar        Articulated
BAU       Business-as-usual scenario
Bi        Bi-articulated, double-articulated
BRL       Brazilian Real
BRT       Bus Rapid Transit
C40       C40 Cities Climate Leadership Group
CD        Charge-depleting
CH4       Methane
CO2       Carbon dioxide
CO2e      Carbon dioxide equivalent
Conv      Conventional
ConvBi    Conventional bi-articulated bus
ConvBiO   Conventional bi-articulated bus — operating in Curitiba
ConvTwO   Conventional two-axle bus — operating in Curitiba
COP       Conference of the Parties
CS        Charge-sustaining
CV        Coefficient of Variation
DSL       Diesel
E01       Technology: Electricity generation from coal
E21       Technology: Electricity generation from nuclear
E31       Technology: Electricity generation from hydro
E51       Technology: Electricity generation from pumped-storage
E70       Technology: Electricity generation from diesel
ELC       Electricity
EU        European Union
GAMS      General Algebraic Modeling System
gCO2      Grams of carbon dioxide
gCO2e,TTW Grams of carbon dioxide emitted in the TTW scope
gCO2e     Grams of carbon dioxide equivalent
gCO2e,WTT Grams of carbon dioxide equivalent expended in the WTT scope
<table>
<thead>
<tr>
<th>Acronym</th>
<th>Description</th>
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<tbody>
<tr>
<td>gCO₂e,WTW</td>
<td>Grams of carbon dioxide equivalent expended and emitted in the WTW scope</td>
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<tr>
<td>GHG</td>
<td>Greenhouse gas</td>
</tr>
<tr>
<td>GNU</td>
<td>GNU operating system and a collection of computer software</td>
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<tr>
<td>GPS</td>
<td>Global Positioning System</td>
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<tr>
<td>GREET</td>
<td>Greenhouse gases, Regulated Emissions, and Energy use in Transportation</td>
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<td>GSL</td>
<td>Petrol (Gasoline)</td>
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<td>GVW</td>
<td>Permitted Gross Vehicle Weight</td>
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<td>GW</td>
<td>Gigawatt</td>
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<td>Hyb</td>
<td>Hybrid-electric</td>
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<td>HYB</td>
<td>Hybrid-electric scenario</td>
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<td>HybAr</td>
<td>Hybrid-electric articulated bus</td>
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<td>HybArA</td>
<td>Hybrid-electric articulated bus — alternative for Curitiba</td>
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<td>HybTw</td>
<td>Hybrid-electric two-axle bus</td>
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<tr>
<td>HybTwA</td>
<td>Hybrid-electric two-axle bus — alternative for Curitiba</td>
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<td>HybTwO</td>
<td>Hybrid-electric two-axle bus — operating in Curitiba</td>
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<td>ICT</td>
<td>Information and Communication Technology</td>
</tr>
<tr>
<td>IEA</td>
<td>International Energy Agency</td>
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<td>IMPDSL1</td>
<td>Technology: diesel import</td>
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<td>IMPGSL1</td>
<td>Technology: petrol import</td>
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<td>IMPHCO1</td>
<td>Technology: coal import</td>
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<td>IMPOIL1</td>
<td>Technology: crude oil import</td>
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<td>IMPURN1</td>
<td>Technology: uranium import</td>
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<tr>
<td>IoT</td>
<td>Internet-of-Things</td>
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<td>IPCC</td>
<td>Intergovernmental Panel on Climate Change</td>
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<td>ITS</td>
<td>Intelligent Transport System</td>
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<tr>
<td>kgCO₂</td>
<td>Kilograms of carbon dioxide</td>
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<td>Kurt</td>
<td>Kurtosis</td>
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<td>kWh</td>
<td>Kilowatt-hour</td>
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<td>L</td>
<td>Litre</td>
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<tr>
<td>LCA</td>
<td>Life cycle assessment</td>
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<td>M$</td>
<td>Million US dollars</td>
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<tr>
<td>MJ</td>
<td>Megajoule</td>
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<td>MJfossil,WT</td>
<td>Megajoule of fossil energy expended in the WTT scope</td>
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<td>MJfossil,WTW</td>
<td>Megajoule of fossil energy expended and consumed in the WTW scope</td>
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<td>Abbreviation</td>
<td>Description</td>
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<tr>
<td>MJ&lt;sub&gt;fuel&lt;/sub&gt;</td>
<td>Megajoule of fuel</td>
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<tr>
<td>MJ&lt;sub&gt;TTW&lt;/sub&gt;</td>
<td>Megajoule of fuel use in the TTW scope</td>
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<td>N</td>
<td>Number of measurements</td>
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<td>N&lt;sub&gt;2&lt;/sub&gt;O</td>
<td>Nitrous oxide</td>
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<tr>
<td>NREL</td>
<td>National Renewable Energy Laboratory, USA</td>
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<td>OSeMOSYS</td>
<td>Open Source energy MOdelling SYStem</td>
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<td>Plug</td>
<td>Plug-in hybrid-electric</td>
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<td>PLUG</td>
<td>Plug-in hybrid-electric scenario</td>
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<td>Plug-in hybrid-electric scenario with management strategy A</td>
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<td>PLUG-B</td>
<td>Plug-in hybrid-electric scenario with management strategy B</td>
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<td>Plug-in hybrid-electric two-axle bus</td>
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<td>Plug-in hybrid-electric two-axle bus — alternative for Curitiba</td>
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<td>PuLP</td>
<td>A Linear Programming Toolkit for Python</td>
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<td>Pyomo</td>
<td>Python Optimization Modeling Objects</td>
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<tr>
<td>Q25</td>
<td>25%-Quantile</td>
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<tr>
<td>Q75</td>
<td>75%-Quantile</td>
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<td>RHE</td>
<td>Technology: Electrical heating</td>
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<td>RHO</td>
<td>Technology: Oil heating</td>
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<td>RL1</td>
<td>Technology: Lightbulbs</td>
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<tr>
<td>RPM</td>
<td>Revolutions per minute</td>
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<td>RTO</td>
<td>Real-time optimisation</td>
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<td>S.D.</td>
<td>Sample standard deviation</td>
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<td>SDG</td>
<td>Sustainable Development Goal</td>
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<tr>
<td>Skew</td>
<td>Skewness</td>
</tr>
<tr>
<td>SOC</td>
<td>State-of-charge</td>
</tr>
<tr>
<td>SOC&lt;sub&gt;high&lt;/sub&gt;</td>
<td>High state-of-charge</td>
</tr>
<tr>
<td>SOC&lt;sub&gt;low&lt;/sub&gt;</td>
<td>Low state-of-charge</td>
</tr>
<tr>
<td>SOC&lt;sub&gt;threshold&lt;/sub&gt;</td>
<td>State-of-charge threshold</td>
</tr>
<tr>
<td>SRE</td>
<td>Technology: Oil refinery</td>
</tr>
<tr>
<td>TAED</td>
<td>Total all-electric distance</td>
</tr>
<tr>
<td>TAET</td>
<td>Total all-electric time</td>
</tr>
<tr>
<td>Short Form</td>
<td>Description</td>
</tr>
<tr>
<td>------------</td>
<td>-------------</td>
</tr>
<tr>
<td>TTW</td>
<td>Tank-to-Wheel</td>
</tr>
<tr>
<td>Tw</td>
<td>Two-axle</td>
</tr>
<tr>
<td>TXD</td>
<td>Technology: diesel vehicles</td>
</tr>
<tr>
<td>TXE</td>
<td>Technology: electric vehicles</td>
</tr>
<tr>
<td>TXG</td>
<td>Technology: petrol vehicles</td>
</tr>
<tr>
<td>UN</td>
<td>United Nations</td>
</tr>
<tr>
<td>US</td>
<td>United States</td>
</tr>
<tr>
<td>USD</td>
<td>US dollar</td>
</tr>
<tr>
<td>WTT</td>
<td>Well-to-Tank</td>
</tr>
<tr>
<td>WTW</td>
<td>Well-to-Wheel</td>
</tr>
</tbody>
</table>
## Glossary

*Table A1: Technical terms (modified and complemented table from Paper II)*

<table>
<thead>
<tr>
<th>Technical term</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>All-electric drive/operation</td>
<td>A bus only uses electricity for driving.</td>
</tr>
<tr>
<td>All-electric range</td>
<td>The distance that a bus can drive only on electricity.</td>
</tr>
<tr>
<td>Accumulated annual demand</td>
<td>This parameter in the OSeMOSYS modelling framework defines the total annual final energy use by all transport-related end-users and is separately provided for each modelled year in the input dataset.</td>
</tr>
<tr>
<td>Articulated bus</td>
<td>An articulated bus is built on a two-section chassis having one pivoting joint and three axles. This chassis has typically a length of around 18 meters and a passenger carrying capacity of 140–170 passengers.</td>
</tr>
<tr>
<td>Bi-articulated bus</td>
<td>A bi-articulated bus — or so-called double-articulated bus — is built on a three-section chassis having two pivoting joints and four axles. This chassis has typically a length of around 25 meters and passenger carrying capacity of 230–250 passengers.</td>
</tr>
<tr>
<td>Big data</td>
<td>Amount of data that typically requires a multi-node cluster database for storage and sometimes a computer cluster for processing.</td>
</tr>
<tr>
<td>Biodiesel blend B7</td>
<td>A fuel blend consisting of 93% petroleum diesel and 7% biodiesel.</td>
</tr>
<tr>
<td>Bus rapid transit (BRT) system/concept</td>
<td>A bus-based transit system concept that provides comfortable, time- and cost-efficient passenger transport at light rail- or metro-level capacities. The BRT concept features include exclusive bus lanes with alignment to the centre of the road, off-board fare collection, platform-level boarding and prioritising of buses over other traffic.</td>
</tr>
<tr>
<td>C40 network</td>
<td>&quot;C40 is a network of the world’s megacities committed to addressing climate change. C40 supports cities to collaborate effectively, share knowledge and drive meaningful, measurable and sustainable action on climate change.&quot; (C40, 2019a)</td>
</tr>
<tr>
<td>Charge-depleting (CD) mode</td>
<td>Operation of a plug-in hybrid-electric bus when more electricity is used than being recovered from the regenerative braking system, i.e. the SOC decreases over distance or time.</td>
</tr>
<tr>
<td>Charge-sustaining (CS) mode</td>
<td>Operation of hybrid-electric and plug-in hybrid-electric buses when the SOC maintains approximately constant due to a sustainable balance between electricity use to drive all-electric and the amount of electricity generated by the regenerative braking system.</td>
</tr>
<tr>
<td>Chassis</td>
<td>A framework for the construction and use of an object, e.g. a bus.</td>
</tr>
<tr>
<td>Chebyshev’s inequality</td>
<td>Description for the spread of data according to the empirical rule that a 1-(1/k^2) proportion of the data is covered by (k) standard deviations.</td>
</tr>
<tr>
<td>Clean bus</td>
<td>Declaration for “low and ultimately zero emission buses” (C40, 2015b).</td>
</tr>
<tr>
<td>Climate target</td>
<td>The goal to limit the global mean temperature rise to well below 2°C compared to pre-industrial levels.</td>
</tr>
<tr>
<td>Conventional powertrain</td>
<td>A propulsion system that employs an internal combustion engine. The only external energy source is liquid fuel.</td>
</tr>
<tr>
<td>Cost of transport service</td>
<td>Total cost per kilometre to operate a bus in a profitable way. The cost of transport service is used as a reference to calculate the fare to the passengers in Curitiba.</td>
</tr>
<tr>
<td>Decarbonisation</td>
<td>The process to decarbonise a system, e.g. reductions of both fossil energy use and the amount of emitted greenhouse gases from urban transport systems.</td>
</tr>
<tr>
<td>Digitalisation</td>
<td>The process to convert information into digital formats so that those can be processed by a computer.</td>
</tr>
<tr>
<td>Driving cycle</td>
<td>A series of data points that represent the speed versus time of a vehicle.</td>
</tr>
<tr>
<td>Elevation profile</td>
<td>A series of data points that represent the road gradient versus distance of a route.</td>
</tr>
</tbody>
</table>
### Table A1: (continued)

<table>
<thead>
<tr>
<th>Technical term</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Hybrid-electric powertrain</td>
<td>A propulsion system that employs both an internal combustion engine and an electric motor for driving. An on-board regenerative braking is used to recover braking energy and convert it into electricity. The only external energy source is liquid fuel.</td>
</tr>
<tr>
<td>Intelligent Transport System (ITS)</td>
<td>A transport concept in which buses use internet connectivity to send and receive information with the aim to enable new services.</td>
</tr>
<tr>
<td>Internal combustion engine</td>
<td>A heat engine that converts heat energy released from fuel combustion in its combustion chamber into mechanical energy.</td>
</tr>
<tr>
<td>Internet-of-Things (IoT)</td>
<td>A system concept in which objects use internet connectivity for information exchange.</td>
</tr>
<tr>
<td>Large data(set)</td>
<td>Amount of data that usually fits in an ordinary database and the capabilities of a single computer are usually sufficient for data processing.</td>
</tr>
<tr>
<td>Life cycle assessment (LCA)</td>
<td>Methodology to assess the environmental impacts in all stages of a product’s life.</td>
</tr>
<tr>
<td>Monte Carlo simulation</td>
<td>An uncertainty analysis method that uses random sampling of input values for parameters.</td>
</tr>
<tr>
<td>Multiprocessing</td>
<td>Use of multiple processes to process simultaneously several data files in parallel.</td>
</tr>
<tr>
<td>Net present cost (NPC)</td>
<td>The NPC states the sum of all costs and revenues, e.g. in an energy system, over the considered time period in an analysis discounted to the first year of the time period.</td>
</tr>
<tr>
<td>Nominal capacity</td>
<td>Amount of electricity that is stored in a fully charged battery.</td>
</tr>
<tr>
<td>Occupancy rate</td>
<td>Passenger carrying capacity utilization rate of a bus, expressed in percentage (%).</td>
</tr>
<tr>
<td>Open data</td>
<td>Data to which access is provided and allows its use and distribution.</td>
</tr>
<tr>
<td>Opportunity charging</td>
<td>Charging concept in which the on-board battery is recharged during the operation day of the plug-in hybrid-electric and/or electric bus.</td>
</tr>
<tr>
<td>Parallel configuration</td>
<td>Capability that both internal combustion engine and electric motor provide simultaneously torque for propulsion in a powertrain.</td>
</tr>
<tr>
<td>Paris Agreement</td>
<td>The agreement that was made at the Conference of the Parties (COP) 21 in Paris to achieve the climate target.</td>
</tr>
<tr>
<td>Passenger carrying capacity (PCC)</td>
<td>Number of passengers that can be transported in a bus.</td>
</tr>
<tr>
<td>Passenger load</td>
<td>Aggregated weight of passengers transported in a bus.</td>
</tr>
<tr>
<td>Passenger-kilometre (pkm)</td>
<td>The functional unit pkm states the aggregated number of passengers travelling together in a transit vehicle, e.g. 20 passengers travelling one kilometre together amounts to 20 pkm.</td>
</tr>
<tr>
<td>Petroleum diesel</td>
<td>Diesel produced from fossil crude oil.</td>
</tr>
<tr>
<td>Plug-in hybrid-electric powertrain</td>
<td>A propulsion system that employs both an internal combustion engine and an electric motor for driving. In addition to regenerative braking, the on-board battery can be recharged with electricity from the power grid at a charging station. The external energy sources are liquid fuel and electricity.</td>
</tr>
<tr>
<td>Powertrain</td>
<td>Components that build the propulsion system of a vehicle.</td>
</tr>
<tr>
<td>Python</td>
<td>An open source interpreted high-level general-purpose programming language.</td>
</tr>
<tr>
<td>Range anxiety</td>
<td>The feeling of fear to not reach the destination due to an insufficient (all-electric) range of a vehicle.</td>
</tr>
<tr>
<td>Range extender</td>
<td>Declaration of an internal combustion engine in a plug-in hybrid-electric powertrain.</td>
</tr>
<tr>
<td>Real-time optimisation (RTO)</td>
<td>A control technique that applies periodic exchange of data and its use in an optimisation model.</td>
</tr>
</tbody>
</table>
Table A1: (continued)

<table>
<thead>
<tr>
<th>Technical term</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Regenerative braking system</td>
<td>An on-board system in a bus that converts excess braking energy into electricity rather than being lost in the form of heat during braking. The electricity is temporary stored in an on-board battery.</td>
</tr>
<tr>
<td>Ridership</td>
<td>Number of passengers travelling in a transport system or on a bus route.</td>
</tr>
<tr>
<td>State-of-charge (SOC)</td>
<td>Ratio of available capacity to the nominal capacity in a battery (full: 100%; empty: 0%). High SOC: Upper limit of the usable capacity in which a battery is used. Low SOC: Lower limit of the usable capacity in which a battery is used. SOC threshold: Threshold at which all-electric operation is stopped.</td>
</tr>
<tr>
<td>Tank-to-Wheel (TTW)</td>
<td>The TTW scope analyses the fuel use during the operation phase of a vehicle.</td>
</tr>
<tr>
<td>Transition technology</td>
<td>A transition technology concerns the transition phase and refers to a technology that can use or support the use of electricity in bus transport systems for passenger transport without relying exclusively on electricity as an energy source for operation. This includes bus technologies as well as tools and models that can support and optimise the transition phase.</td>
</tr>
<tr>
<td>Two-axle bus</td>
<td>A two-axle bus is built on a single-section chassis having two axles. This chassis has typically a length of around 12 meters and a passenger carrying capacity of 70–90 passengers.</td>
</tr>
<tr>
<td>Well-to-Tank (WTT)</td>
<td>The WTT scope analyses the fuel production and supply of a transport fuel.</td>
</tr>
<tr>
<td>Well-to-Wheel (WTW)</td>
<td>The combined consideration of the WTT scope and TTW scope.</td>
</tr>
</tbody>
</table>
### Sustainable Development Goals

The thesis' objective intends to contribute to the following selected SDGs and selected targets (UN, 2018). The particular contributions are highlighted in bold font:

- **SDG 3: Good health and well-being**
  - Target 3.9: “By 2030, substantially **reduce** the number of deaths and illnesses from hazardous chemicals and **air**, water and soil **pollution** and contamination”
  - Target 3.9.1: “**Mortality rate attributed to household and ambient air pollution**”

- **SDG 7: Affordable and clean energy**
  - Target 7.3: “**By 2030, double the global rate of improvement in energy efficiency**”

- **SDG 11: Sustainable cities and communities**
  - Target 11.2: “**By 2030, provide access to safe, affordable, accessible and sustainable transport systems for all, improving road safety, notably by expanding public transport, with special attention to the needs of those in vulnerable situations, women, children, persons with disabilities and older persons**”
  - Target 11.3: “**By 2030, enhance inclusive and sustainable urbanization and capacity for participatory, integrated and sustainable human settlement planning and management in all countries**”
  - Target 11.6.2: “**Annual mean levels of fine particulate matter (e.g. PM2.5 and PM10) in cities (population weighted)**”

- **SDG 13: Climate action**
  - Target 13.2: “Integrate **climate change measures** into national policies, strategies and planning”
  - Target 13.2.1: “**Number of countries that have communicated the establishment or operationalization of an integrated policy/strategy/plan which increases their ability to adapt to the adverse impacts of climate change, and foster climate resilience and low greenhouse gas emissions development in a manner that does not threaten food production (including a national adaptation plan, nationally determined contribution, national communication, biennial update report or other)**”


References | 85


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