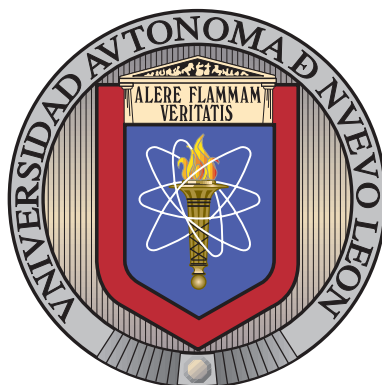


UNIVERSIDAD AUTÓNOMA DE NUEVO LEÓN

FACULTAD DE CIENCIAS FÍSICO MATEMÁTICAS



MATHEMATICAL PROGRAMMING FOR
STRATEGIC DECISION-MAKING IN PUBLIC
TRANSPORT SYSTEMS

POR

KARLA ISABEL CERVANTES SANMIGUEL

EN OPCIÓN AL GRADO DE
DOCTOR EN CIENCIAS
CON ORIENTACIÓN EN MATEMÁTICAS

SAN NICOLÁS DE LOS GARZA, NUEVO LEÓN

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Facultad de Ciencias Físico Matemáticas

Los miembros del Comité de Tesis recomendamos que la Tesis “Mathematical Programming for Strategic Decision-Making in Public Transport Systems”, realizada por la alumna Karla Isabel Cervantes Sanmiguel, con número de matrícula 1620533, sea aceptada para su defensa como opción al grado de Doctor en Ciencias con Orientación en Matemáticas.

El Comité de Tesis

Dr. Omar Jorge Ibarra Rojas
Director

Dra. María Victoria Chávez Hernández
Revisor

Dr. Ricardo Giesen
Revisor

Dr. Álvaro Eduardo Cordero Franco
Revisor

Dr. José Guadalupe Flores Muñiz
Revisor

Vo. Bo.

Dr. Omar Jorge Ibarra Rojas
Coordinador del Posgrado en Ciencias con
Orientación en Matemáticas

San Nicolás de los Garza, Nuevo León, Diciembre 2025

*To my parents, Isabel and Carlos,
my brothers, Jair and Alan,
my inspiration, Luis Angel,
and our joy, Kiper
with all my love.*

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ABSTRACT

This doctoral thesis explores the application of operations research techniques to improve the performance and sustainability of public transport systems. The research is structured around two complementary studies that address critical challenges in the planning and management of public transport networks: (i) the estimation of Origin-Destination Matrices (ODMs) from heterogeneous data sources, and (ii) the sustainable planning of bus fleet replacement under economic, environmental, and social objectives.

In the first part of this thesis, we address the problem of estimating public transport ODMs by developing a series of bi-level optimisation models that integrate different types of information, including outdated matrices, observed passenger flows, and boarding and alighting data. These models are reformulated into single-level mathematical programmes and solved using commercial solvers on benchmark instances. The results demonstrate that the inclusion of multiple data types significantly improves estimation accuracy, and provide valuable insights into the role of data availability and structure in transport demand modelling.

The second part focuses on the transition towards sustainable public transport systems by proposing a multi-objective optimisation model for the replacement of diesel bus fleets with electric vehicles. The model determines the timing, quantity, and type of vehicles to purchase, as well as their optimal allocation across bus lines, under budgetary and operational constraints. The objectives include minimising total costs, maximising fleet electrification, and promoting equity in vehicle distribution across different city regions. An epsilon-constraint algorithm is implemented to approximate the Pareto front and reveal the trade-offs between the competing goals of economic efficiency, environmental impact, and social equity.

Together, these two studies contribute to the field of public transport optimisation by providing novel mathematical formulations, computational approaches, and policy-relevant insights. The thesis advances the understanding of how data-driven optimisation can enhance both the operational efficiency and sustainability of urban transport systems,

offering practical tools and analytical frameworks for decision-makers in the transition towards more intelligent and equitable mobility.

Keywords: public transport optimisation, Origin-Destination Matrix estimation, bi-level programming, multi-objective optimisation, sustainable mobility, electric bus fleets, operations research.

CHAPTER 1

INTRODUCTION

1.1 CONTEXT

Efficient and accessible public transportation systems are fundamental pillars of sustainable urban development. Mobility plays a central role in the quality of life of citizens, influencing access to employment, education, healthcare, and social opportunities. As urban populations continue to grow, the reliance on private vehicles has intensified, resulting in increased traffic congestion, air pollution, and greenhouse gas emissions. This trend underscores the urgent need to strengthen public transport systems, not only to alleviate congestion but also to reduce environmental impacts and improve urban well-being. Investing in high-quality public transportation generates benefits that extend beyond mobility, contributing to economic productivity, environmental protection, social equity, and public health (Tumlin, 2012).

Designing and operating an efficient public transport system is a complex task that typically involves a structured sequence of decision-making problems, including network design, frequency setting, timetable design, and fleet and crew scheduling (Ceder and Wilson, 1986). These planning stages operate at different decision levels, strategic, tactical, and operational, and involve trade-offs among cost efficiency, service quality, and environmental performance (Desaulniers and Hickman, 2007; Ibarra-Rojas et al., 2015). The interdependence of these stages and the heterogeneity of available data make comprehensive optimisation approaches both challenging and essential. As such, research in this field often focuses on specific strategic components that can substantially enhance the performance and sustainability of transit systems (see Figure 1).

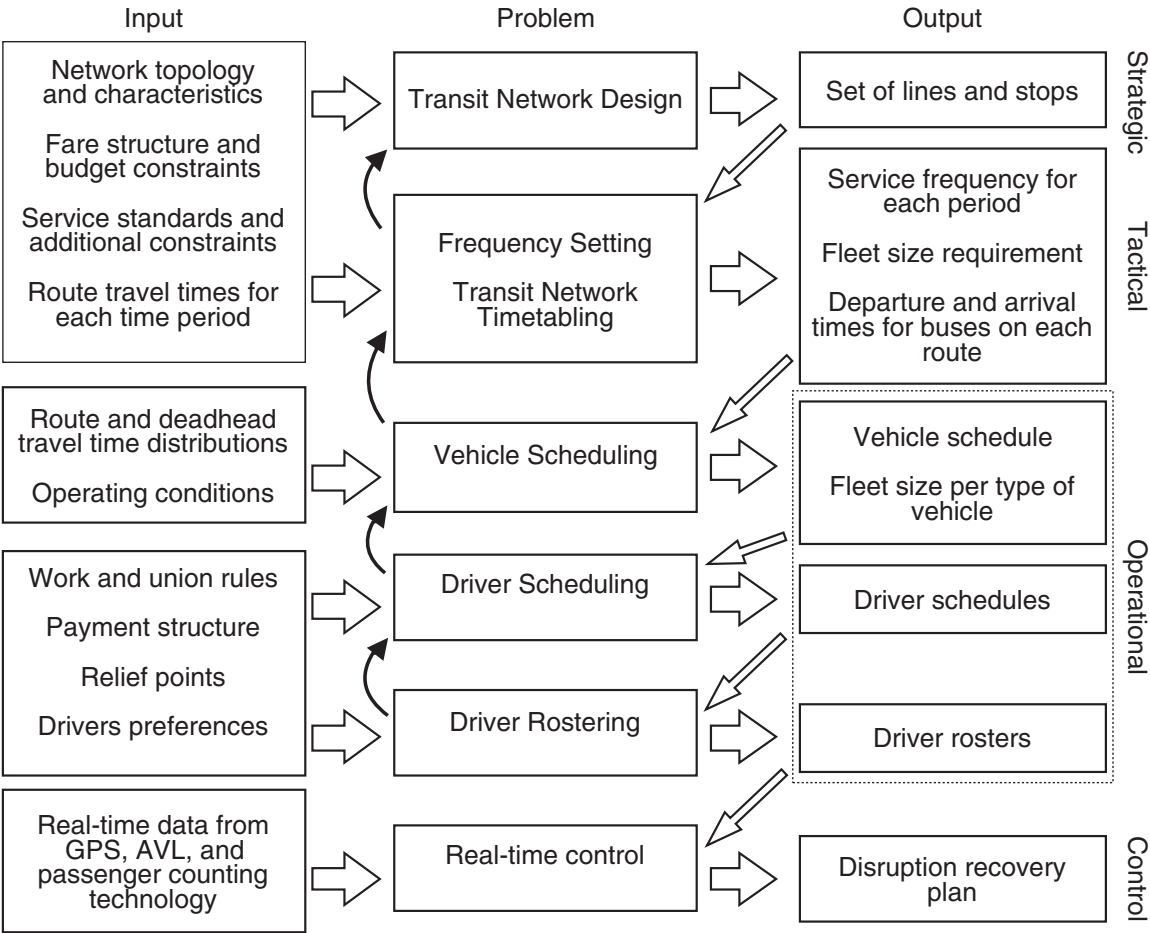


Figure 1: Decision levels in public transport planning and their associated problem. Source: Ibarra-Rojas et al. (2015).

This research focuses on two strategic-level problems that arise once the transit system is already established and operational. At this stage, the network structure and main service design decisions are in place, and the emphasis shifts towards enhancing system performance through data-driven analysis and long-term planning (see Figure 2).

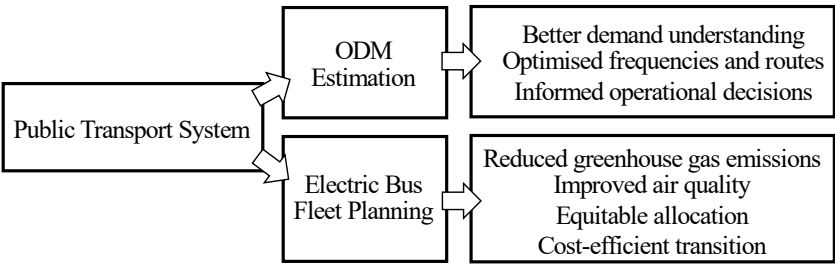
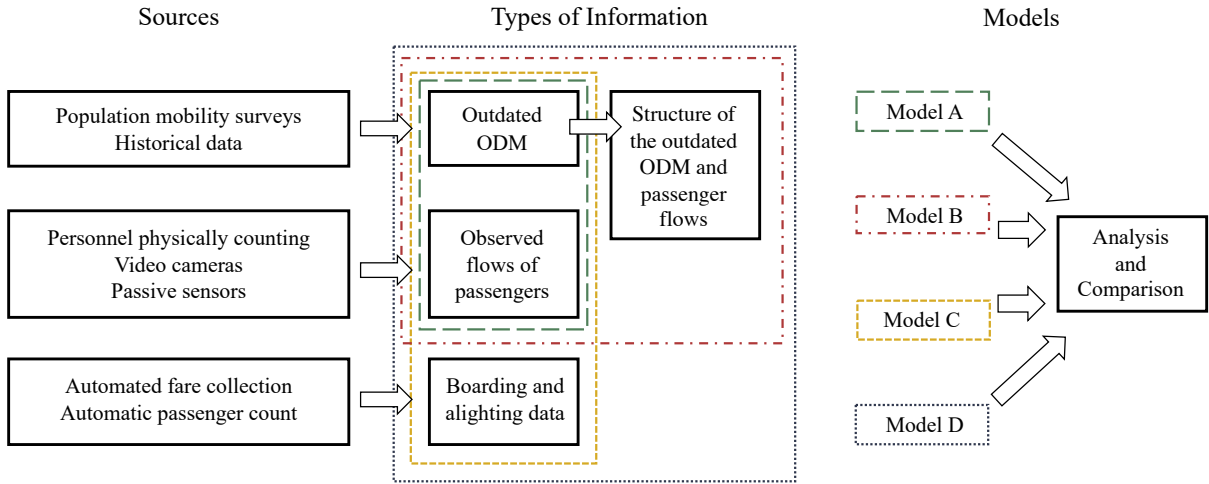


Figure 2: Strategic-level decisions and benefits in public transport.

Within this context, this research addresses two strategic-level problems that contribute to improving public transport planning and operation through optimisation-based methodologies. The first research project focuses on estimating passenger demand in transit networks by developing different mathematical models for origin-destination (OD) matrix estimation using various data sources that provide different types of information such as boarding/alighting counts, passenger flows, and outdated OD matrix data (see upper panel in Figure 3). The second project introduces a multi-objective optimisation framework for planning the sustainable replacement of diesel bus fleets with electric vehicles in a multi-year planning horizon, optimising economic, environmental, and social objectives, leading to a sustainable approach of public transport (see lower panel in Figure 3).

(a) OD Matrix estimation
Sources



(b) Sustainable bus replacement

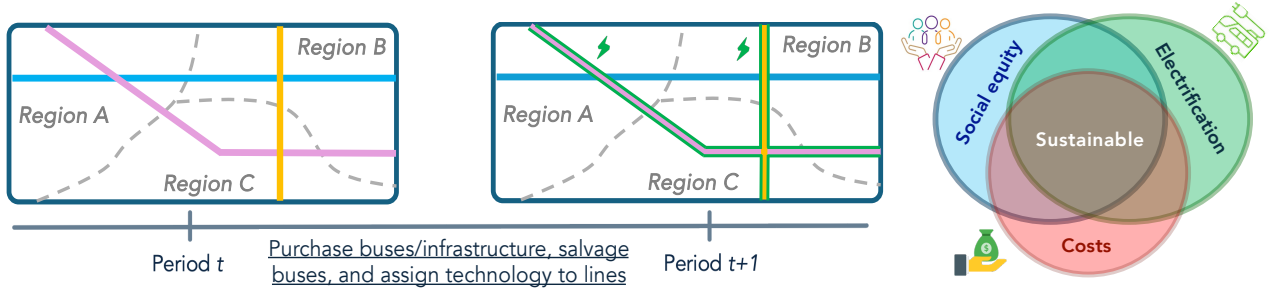


Figure 3: Optimisation approaches of this study.

Based on the above, our goal is to provide handy tools for strategic planning in public transport. In particular, by implementing mathematical programming techniques to model relevant decision-making problems in transportation, taking advantage of trending technologies and available data, as well as propose efficient solution algorithms capable

of generate high-quality solutions in acceptable computational times. We now formally introduce the research objectives of this study.

1.2 RESEARCH OBJECTIVES

The overarching objective of this doctoral research is to develop and analyse optimisation-based models that enhance the efficiency and sustainability of public transport systems. This thesis integrates two complementary studies: one focused on improving the estimation of passenger demand through origin-destination (OD) matrices, and another dedicated to supporting the transition towards sustainable bus fleets. Together, these models aim to provide decision-makers with robust, data-driven tools for optimising both operational performance and long-term environmental goals.

1.2.1 GENERAL OBJECTIVE

The general objective of this research is to formulate and evaluate optimisation models that contribute to sustainable public transport planning by:

- Enhancing the accuracy of OD matrix estimation using multiple types of passenger data, and
- Designing multi-objective strategies for electric bus fleet replacement that balance economic, environmental, and social considerations.

1.2.2 SPECIFIC OBJECTIVES

The specific objectives of this doctoral research are to:

1. Study public transport systems to identify optimisation opportunities that improve service efficiency and sustainability, particularly in demand estimation and fleet management.
2. Develop mathematical formulations for two interrelated problems: (i) bi-level optimisation models for estimating OD matrices from heterogeneous data sources, and (ii) a multi-objective optimisation model for electric bus fleet replacement and allocation.
3. Implement computational solution methods, including single-level reformulations and the epsilon-constraint algorithm, and assess their performance on benchmark instances.

4. Investigate the trade-offs among the objectives in both models such as data use versus accuracy in OD estimation, and cost versus equity and emissions reduction in fleet planning.
5. Derive practical recommendations for transport authorities to support evidence-based, equitable, and sustainable decision-making in public transport planning.

1.3 METHODOLOGY

The research develops and applies optimisation-based approaches to address two distinct challenges in public transportation planning. For origin-destination matrix estimation, bi-level models are formulated to account for combinations of outdated matrices, observed passenger flows, boarding and alighting data, and network structural characteristics. These models are reformulated into single-level optimisation problems and solved using commercial solvers across benchmark instances to evaluate the impact of different information types on estimation accuracy. In the context of sustainable bus fleet replacement, a multi-objective optimisation framework determines the timing, quantity, and allocation of electric vehicles, incorporating economic, environmental, and social criteria. An ε -constraint algorithm is employed to approximate the Pareto front, facilitating the analysis of trade-offs among objectives. Computational experiments and sensitivity analyses are conducted to assess model performance, explore the influence of input parameters, and provide insights for strategic decision-making.

1.4 SCIENTIFIC CONTRIBUTIONS

This doctoral research makes several scientific contributions to the field of public transport optimisation and sustainable mobility planning. These contributions span methodological, analytical, and practical aspects, addressing two major challenges in urban transport systems: (i) the accurate estimation of passenger origin-destination (OD) matrices using diverse data sources, and (ii) the sustainable replacement and allocation of bus fleets under multiple objectives. The key contributions are summarised as follows:

1. *Novel optimisation models for OD matrix estimation.* This thesis introduces a set of bi-level optimisation models designed to estimate public transport OD matrices by integrating multiple data types, including outdated OD matrices, passenger flow data, and boarding-alighting information. The models are reformulated into single-level problems, allowing their solution with a standard commercial solver. This

approach provides a systematic framework to evaluate how different data combinations affect the accuracy of OD matrix estimation, an aspect that has received limited attention in previous research.

2. *Comprehensive analysis of data-driven estimation accuracy.* Through numerical experiments, this research quantifies the impact of various data inputs on model performance and accuracy. The analysis reveals the importance of data selection and the interactions between different data sources, offering valuable insights for transport agencies aiming to improve demand estimation with limited or heterogeneous datasets.
3. *A multi-objective optimisation framework for sustainable fleet planning.* A new multi-objective model is developed to guide the replacement of diesel bus fleets with electric vehicles. The model simultaneously minimises total costs, including acquisition, maintenance, energy, and infrastructure costs, while maximising fleet electrification and promoting equity across city regions. This comprehensive formulation captures the economic, environmental, and social dimensions of sustainable transport planning within a unified optimisation framework.
4. *Application of the epsilon-constraint method for Pareto front approximation.* The proposed model applies the epsilon-constraint algorithm to generate a representative set of non-dominated solutions, allowing a detailed exploration of trade-offs among competing objectives. This methodological contribution enhances decision support by providing transport planners with alternative optimal strategies reflecting different policy priorities.
5. *Integration of optimisation insights for decision-making.* Beyond individual models, this research synthesises findings across both projects, demonstrating how optimisation techniques can inform data-driven and sustainability-oriented decision-making in public transport planning. The results contribute to bridging the gap between theoretical modelling and practical implementation, supporting more resilient and equitable urban transport systems.

In summary, this thesis advances the understanding of how optimisation methods can be employed to tackle key challenges in public transport management. It provides methodological innovations, analytical insights, and decision-support tools that contribute to both the academic literature and real-world transport policy design.

1.5 THESIS STRUCTURE

This thesis is structured to systematically present the research conducted on public transport demand estimation and sustainable bus fleet planning. Chapter 1 presented the context, research objectives, methodology, and key scientific contributions. Chapter 2 reviews the relevant literature on origin-destination matrix estimation and electric bus fleet transition, highlighting the gaps addressed by this work. Chapter 3 details the bi-level optimisation models for estimating public transport OD matrices, including their formulation, computational approach, and analysis of results. Chapter 4 develops a multi-objective framework for sustainable bus fleet replacement, addressing economic, environmental, and social objectives, and presenting solution methods and managerial insights. Chapter 5 summarises the main findings, discusses implications, and outlines directions for further research. Supporting analyses and additional computational details are provided in the appendices.

CHAPTER 2

RELATED LITERATURE

Urban public transport systems are the focus of extensive research due to their critical role in ensuring mobility, reducing environmental impacts, and promoting social equity. In this context, two complementary strands of literature are particularly relevant to this thesis. The first concerns the estimation of origin-destination matrices (ODMs), which are essential for understanding passenger travel patterns and informing operational decisions such as line frequencies and network design. The second strand focuses on the planning and optimisation of bus fleet transitions, particularly the replacement of diesel buses with electric vehicles, considering multi-objective criteria including cost, environmental impact, and equitable service distribution. This section reviews both bodies of literature separately, highlighting methodological advances, key findings, and the context in which each project of this thesis is situated. By examining these two strands, we establish the foundation for the subsequent chapters, which present the original contributions of this research.

2.1 ORIGIN-DESTINATION MATRIX ESTIMATION

Historically, ODMs were obtained from passenger surveys, which are usually infrequent due to their high cost (Bera and Rao, 2011). In recent years, technological advances have facilitated the acquisition of data through various automatic data collection systems, such as Automatic Vehicle Location (AVL), Automatic Passenger Counting (APC), and Automated Fare Collection (AFC) systems (Mohammed and Oke, 2023). Consequently, researchers have focused their efforts on the ODMs estimation by incorporating easily obtainable information. Our literature review draws on methodologies to estimate an ODM for public transport systems that utilise different types of data, allowing us to highlight the context and contributions of our study effectively. Table 1 summarises the type of information used in each study reviewed and emphasises the analysis of the impact of different data types on the estimated ODM.

Study	Outdated information			Updated information		
	ODM	ODM structure	Pax flows structure	Observed flows	Alighting data	Boarding data
Lam et al. (2003)	✓		✓	✓		
Wu and Lam (2006)	✓		✓	✓		
Chávez-Hernández et al. (2019)	✓			✓		
Barry et al. (2002)						✓
Alsger et al. (2015)						✓
Sánchez-Martínez (2017)						✓
Hamedmoghadam et al. (2021)						✓
Liu et al. (2021)					✓	✓
Kumar et al. (2019)				✓	✓	✓
Ait-Ali and Eliasson (2022)				✓	✓	✓
Our study	✓	✓	✓	✓	✓	✓

Table 1: Related studies for Origin-Destination matrix estimation for public transport.

As shown in Table 1, common studies typically utilise outdated ODMs and passenger flow structures. However, they also incorporate recent information, such as observed flows along specific arcs in the transit network. For instance, Lam et al. (2003) proposed a bi-level model to estimate ODMs where the lower level corresponds to a frequency-based stochastic user equilibrium assignment model with decisions of line frequencies. Wu and Lam (2006) introduced a bi-level program that optimises error measurements in observed flows and ODM at the upper level while addressing a stochastic user equilibrium assignment in the lower level based on a frequency-adaptive congested transit network model. The researchers suggested a heuristic solution algorithm, although they noted that its applicability to large transit networks might be limited in practice. Lastly, Chávez-Hernández et al. (2019) developed an augmented Lagrangian model and an iterative solution method to deliver high-quality solutions with reduced CPU times. They tested this approach on the Winnipeg and Valley of Mexico transit networks, finding that the elimination of pairs with no demand in the outdated ODM notably reduced computational times.

Regarding the ODM estimation for public transport using only new information, common inputs include boarding counts. For example, Barry et al. (2002) employed New York City Transit’s MetroCard data to determine trip sequences and origin stations, assuming that passengers frequently return to their previous destination station and conclude their day where it started. They found these assumptions valid for 90% of subway users, validating the methodology through exit counts and trip assignment modelling. Alsger et al. (2015) introduced an algorithm to generate matrices from user transactions using Brisbane, Australia’s smart card data, testing the assumptions’ effects regarding walking

distance and transfer times on the ODM. The findings indicated a minimal impact on the estimated ODM with varying transfer time assumptions, with most passengers returning to their initial origin within 800 metres on the same day. Sánchez-Martínez (2017) proposed a dynamic programming model considering various factors, such as waiting time, in-vehicle time, and transfers, in inferring destinations. This model, now employed in Boston, Massachusetts, surpasses earlier models in accuracy. Hamedmoghadam et al. (2021) developed a procedure that utilises statistical pattern recognition to enhance the inference of alighting transactions and identification of transfers. They used smart card data from Melbourne’s multi-modal public transport network to estimate the ODM accurately. Additionally, Liu et al. (2021) included both boarding and alighting data, stating that ODM estimation methods at the route level cannot generalise to the transit network level if relying solely on AVL or APC data. They emphasised the necessity of estimating ODMs in transit networks using AVL/APC data by inferring transfers.

Besides boarding and alighting data, Kumar et al. (2019) and Ait-Ali and Eliasson (2022) employed non-linear program and used Lagrangian relaxation, including observed flows. Specifically, Kumar et al. (2019) utilised a solver and an algorithm to find good-quality solutions for a sparse ODM, where the errors remained within a small range, and as matrix sparsity increased, the method yielded more precise results. Meanwhile, Ait-Ali and Eliasson (2022) evaluated how the accuracy of estimated matrices improved with the inclusion of additional data on link flow, destination count, and average travel distance, starting from origin counts only. They reported that link flows are more challenging to estimate than exit flows; relying solely on entry and exit data is insufficient for precise link flow estimation; average trip distance enhances estimation accuracy; the value of additional destination counts diminishes slowly, justifying the need for more exit station observations; and adding link flow data for some links has minimal impact, especially when other data are already considered.

In contrast to previous approaches, our work introduces multiple decision bi-level models for ODM estimation. Our key contribution, as highlighted in Table 1, differs from prior research in several ways. Firstly, we focus on the structure of the outdated ODM, which has received limited attention in previous studies. Additionally, we conduct our research in the context of public transport, which directly impacts our assignment problem, addressing specific passenger actions such as waiting, travelling, and transferring; we also consider factors such as the frequency of each line and bus capacity. Finally, we assess the impact of various combinations of data types on the estimated Origin-Destination matrix.

The accurate OD matrices produced through these methodologies serve as critical inputs for the second strand of our literature review: optimising electric fleet transitions under multi-criteria objectives.

2.2 ELECTRIC BUS FLEET REPLACEMENT

Operations research techniques such as mathematical programming models have been extensively applied to determine the optimal composition of the fleet for a multi-period planning horizon. These models aim to minimise total system costs while adhering to constraints such as fleet capacity, vehicle life expectancy, and operational requirements (e.g., Emiliano et al., 2020b). On the other hand, the electrification of public transportation networks is a key strategy to reduce greenhouse gas emissions and improve urban air quality, and in the electric bus planning process (strategic, tactical, and operational), various challenges arise. These include: 1) allocation of investments for the electric bus fleet and charging infrastructure, 2) determining optimal locations for charging infrastructure, 3) addressing the scheduling of electric vehicles, and 4) managing the problem of scheduling battery charges (Perumal et al., 2022).

In particular, the assignment of trips to different types of electric buses plays a crucial role in optimising the operational and environmental performance of public transportation systems. Emiliano et al. (2020a) address this problem by formulating a model that optimises a weighted sum of emissions and total costs. Their experimental results highlight the inherent trade-off between economic and environmental objectives. Similarly, Tang et al. (2023) explore the problem of bus selection for a single transit line, integrating vehicle scheduling decisions under the assumption that all buses are replaced simultaneously. This assumption simplifies the optimisation process, but also underscores the importance of considering fleet heterogeneity and gradual replacement strategies in real-world applications. These studies emphasize that bus assignment decisions are not only influenced by cost and environmental factors, but also by operational constraints and long-term fleet renewal strategies, making them a key component in sustainable transit planning. Finally, sensitivity analysis such as that presented in Feng and Figliozzi (2014) plays a crucial role in the evaluation of different replacement policies and parameters under uncertainty. In particular, variations in energy prices, advances in battery technology, and future policy changes have recently been studied for a more efficient adoption of electromobility (see Laboratory, 2016).

Our review of the literature focuses on fleet transition problems considering electric buses and implementing operations research techniques in a multi-period framework that provides valuable information to decision makers.

Various research studies have examined the issue of fleet replacement within the framework of moving toward sustainable public transportation systems. Li et al. (2018) present a problem that aims to maximise the total net benefit of early replacement, where both the optimal size and the composition of the fleet can be determined under budget constraints. The authors formulate the problem as an integer programming model, which is solved using CPLEX for a real-world scenario in Hong Kong. In addition, a sensitivity analysis is conducted to examine the impact of the recharging scheme and the purchase price of buses. Islam and Lownes (2019) focus on minimising the total life cycle cost of fleet replacement while ensuring annual emission reductions and meeting minimum electrification targets. Their mixed-integer programming (MIP) model, implemented using a commercial solver in a case study in Connecticut, USA, highlights the computational efficiency of their approach and its ability to perform sensitivity analyses for evaluating policy implications. Similarly, Pelletier et al. (2019) develop an MIP framework to support fleet electrification on a long-term planning horizon of 30 years. Their model optimises a weighted sum of costs while incorporating constraints related to trip compatibility, maximum vehicle age, and power and space limitations in depots. Applied to a real-world case in France, their results indicate that the model can effectively identify the most suitable fleet types for short- and medium-term planning, as well as assess mid-term cost variations due to factors such as battery replacement.

More recently, Tang et al. (2021) have addressed the fleet replacement problem by considering different electric bus technologies and optimising a weighted total that includes electrification expenses, emission costs, and a measure of user crowdedness. Their mixed-integer non-linear programming (MINLP) model accounts for budget constraints, minimum usage of purchased buses, and maximum bus age. Implemented in a case study in Qingdao, China, their results highlight the influence of social considerations in fleet renewal decisions, demonstrating that cost minimization alone may not be sufficient when designing sustainable and user-friendly public transport systems. Finally, Zhou et al. (2023) proposed an MIP model to optimise the progressive renewal of bus fleets, considering not only economic costs, but also costs of climate, health, and battery recycling. Their model incorporates government incentives as a decision variable and includes key constraints such as bus conservation, charger demand, and charge conservation. Tested on a real-world scenario in Singapore, their approach demonstrates the applicability of the model to the evaluation of different policy incentives. Collectively, these studies underscore the potential of operations research techniques to address the fleet replacement

problem, including a wide range of economic, operational, environmental, and social constraints, making them valuable tools to support decision-making in the planning of sustainable public transportation.

2.3 SUMMARY OF THE LITERATURE REVIEW

The literature reviewed in this chapter highlights the diversity and complexity of research on urban public transport systems. The first strand demonstrates how ODM estimation techniques have evolved from classical statistical models to more advanced optimisation and data-driven approaches, enhancing the accuracy and applicability of travel demand representation. The second strand underscores the growing emphasis on sustainable fleet management, where multi-objective optimisation plays a vital role in achieving trade-offs between cost efficiency, environmental performance, and social equity.

By consolidating insights from both areas, this review provides a comprehensive background that informs the two independent yet complementary projects developed in this thesis. The subsequent chapters build upon these foundations, presenting the proposed optimisation models, their implementation, and the resulting analyses in detail.

CHAPTER 3

OPTIMISATION MODELS FOR ESTIMATING PUBLIC TRANSPORT OD MATRICES USING DIFFERENT DATA TYPES

Understanding how passengers move through an urban public transport network is fundamental for efficient planning and operation. Origin-destination matrices (ODMs) provide a detailed representation of these travel patterns, serving as a cornerstone for service design and optimisation. However, obtaining accurate and up-to-date ODMs remains a challenge due to limitations in available data and the cost of large-scale surveys. This chapter presents optimisation-based models for estimating ODMs using multiple data sources and information types. By formulating the estimation problem as a series of bi-level programmes that are later reformulated into single-level models, we explore how incorporating various data types, such as outdated ODMs, passenger flows, and boarding and alighting counts, affects estimation accuracy. The analysis provides insight into the value of different data combinations and highlights the importance of information structure in improving the reliability of ODM estimations.

3.1 ESTIMATING PASSENGER DEMAND IN PUBLIC TRANSPORT NETWORKS

Origin-Destination (OD) demand matrices provide information about how passengers travel between different zones using a transportation network. This information serves as input for other decision problems in transit network planning, such as transit network design, frequency setting, and timetable design (Ibarra-Rojas et al., 2015). However, estimating an OD matrix (ODM) is a complex task, but it is possible to obtain an approximation by using data obtained from various sources of information.

For example, historical data and population surveys can provide an outdated ODM, while personnel physically counting, video cameras, and/or passive sensors can yield observed passenger flows along transit lines. Additionally, Automated Fare Collection (AFC) and Automated Passenger Count (APC) systems can offer boarding and alighting data (see Figure 4). This variety of information aids in the development of optimisation models. Moreover, recollecting and analysing different sources of information is time-consuming, and it is not simple.

We are interested in alternative approaches to the laborious and expensive process of obtaining data through population surveys, typically conducted every 1 or 2 decades. For example, the literature on estimating ODMs from traffic counts (observed flows) has been extensive (see Bera and Rao, 2011). In particular, Cascetta and Nguyen (1988) presented a methodology for estimating ODMs from traffic counts using a generic traffic assignment map; they showed that the approach is also valid for transit networks with an appropriate assignment map. However, no method is universally accepted as the best because the efficiency of implementing each method depends on factors such as the network size and behaviour, complexity of the proposed methodology, availability of data, and the desired level of accuracy. In response, we propose different and new bi-level optimisation models for ODM estimation considering different types of information.

Our major goal is to identify the information types with the most significant impact on the quality of the generated ODM. In particular, we use the following types of information:

1. An outdated ODM (alternatively called sample, target, prior or obsolete matrix) contains information about travel between different locations but does not provide accurate data on travel patterns. It is obtained using historical data or population mobility surveys and does not reflect changes in how people travel that may have occurred since collecting that data. We also examine the structure of the outdated ODM (also called skeleton) and passenger flows (alternatively known as link probabilities) by assuming a specific passenger travel behaviour, i.e., considering a particular assignment problem (see Behara et al., 2020). We consider proportions; for example, the demand proportion can be represented by the ratio of demand for a specific OD pair to the total demand in the transit network, while passenger flow proportions can be seen as the ratio of the number of passengers for an OD pair using a specific segment of a transit line with respect to the total number of passengers of that OD pair. Indeed, the passenger flow proportions can be seen as the skeletal framework of the ODM, representing the preferences of passengers. This type of data can be obtained directly from the outdated ODM by solving an as-

signment problem to identify the used routes and will be used to guide optimisation models (see Behara et al., 2022; Hussain et al., 2022). The use of this information shows how passengers are distributed across the system for different origin and destination pairs, and we will use these passenger volumes as a reference to guide our optimisation model.

2. Observed flows of passengers travelling on a bus through a specific segment of a transit line (also known as traffic counts, link volumes, segment flows), which can be obtained from manual and automated techniques. Manual methods involve personnel physically counting and recording the number of passengers passing a specific location, whereas automated methods may use technologies such as video cameras or passive sensors to collect data automatically (see Chávez-Hernández et al., 2019; Lam et al., 2003; Pamula and Zochowska, 2023).
3. Boarding and alighting data (or production and attraction zone data) are information about the number of passengers who board/alight a vehicle of a transit line at specific stops. This can be automatically collected through AFC and APC systems (e.g., Kumar et al., 2019; Mohmmad et al., 2023). In general, it is easier to obtain boarding counts than alighting, but our methodology remains for any kind of passenger count at stops.

The efficiency of a method to estimate an ODM depends on the different types of information and how the information is used. In this study, we propose a comparison of new bi-level optimisation models to estimate an ODM based on different data types. Our experimental results lead us to identify the data type with the most significant effect on ODM estimation in multiple scenarios with different demand behaviours. Figure 4 exhibits a scheme of our methodology for ODM estimation.

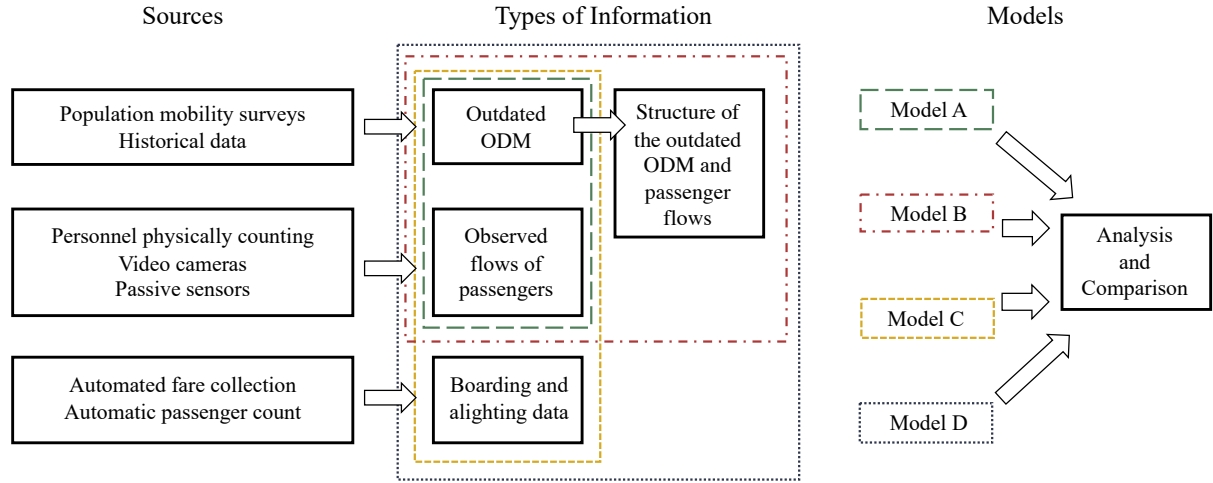


Figure 4: Proposed approach to evaluate optimisation models to estimate an ODM using different types of information.

In summary, this study addresses the estimation of passenger demand at a strategic level of public transport planning, once the transit network is already established. The proposed optimisation-based approach provides a structured framework to analyse how different data sources, such as outdated OD matrices, observed flows, and boarding and alighting information, affect the accuracy of OD matrix estimation. This formulation contributes to improving demand modelling and also enhances the quality of data-driven decision-making processes that support subsequent stages of public transport planning, such as network design and service frequency optimisation.

3.2 BI-LEVEL PROGRAMMING FORMULATIONS FOR THE ODME

As it is mentioned above, we could use different sources of information to generate an ODM for public transport networks; thus, we define several decision problems in terms of the input type. In general, to define our bi-level optimisation problems, we consider a given network, an outdated ODM, and different types of information, such as observed flow for some arcs of the network, the ODM structure, outdated flow proportions, and observed demand in specific stops. Then, our **ODME** problems determine an estimated ODM to minimise a weighted sum of the distance between the generated ODM and the outdated one and the distance between generated flows and outdated flows in the upper level, while the lower level solves the transit assignment problem minimising the total

travel time taking into account the capacity of the buses. In particular, each variant of our problem is defined in terms of the information assumed as an input.

We define the following notation for our ODME problems. Let $G^L = (N^L, A^L)$ be a transit network, where N^L is the set of stops and A^L is the set of arcs (see left panel of Figure 5). Suppose L is the set of lines with frequencies f_l (fixed for the planning period), and $l(a)$ is the line associated with each arc $a \in A^L$. We assume known travel times c_a for each arc $a \in A^L$. Besides, we consider a transit vehicle (bus, train, or other) with a capacity of q pax/veh, and we define K as the set of OD pairs (o_k, d_k) . To represent the upper and lower level of our problem, we use the modelling approach proposed by Cervantes-Sanmiguel et al. (2023), which identifies passenger actions such as waiting for the first bus, performing transfers, waiting to transfer, and travelling by bus. The latter approach takes the lines network G^L as input, and then, it generates an extended network as $G = (N, A)$, where N is the set of stops N^L union with dummy nodes created to model transfer events or compute waiting times. In the case of the arcs, set A represents the union of waiting (A^W), transfer (A^T), and travel (A^V) arcs, where $t(a) \in A^T$ represents the same physical travel trajectory as arc $a \in A^V$, but after travelling along that trajectory, passengers transfer to another line for the next leg of their trip. Note that the travel and transfer arcs ($a \in A^V \cup A^T$) represent segments of the line $l(a)$. Therefore, the flow passing through these arcs represents passengers on a bus of the line $l(a)$. Furthermore, it is important to highlight that information such as the set of bus lines, service frequencies, arc capacities, OD pairs, travel times, and the exclusive associations of each arc to a single bus line in the extended network G are inherited from the lines network G^L . For further insights into the network generation process, please refer to Cervantes-Sanmiguel et al. (2023). Figure 5 represents the modelling approach for the extended network $G = (N, A)$, where it can be noticed that the different arcs represent the different actions of passengers in the transit system.

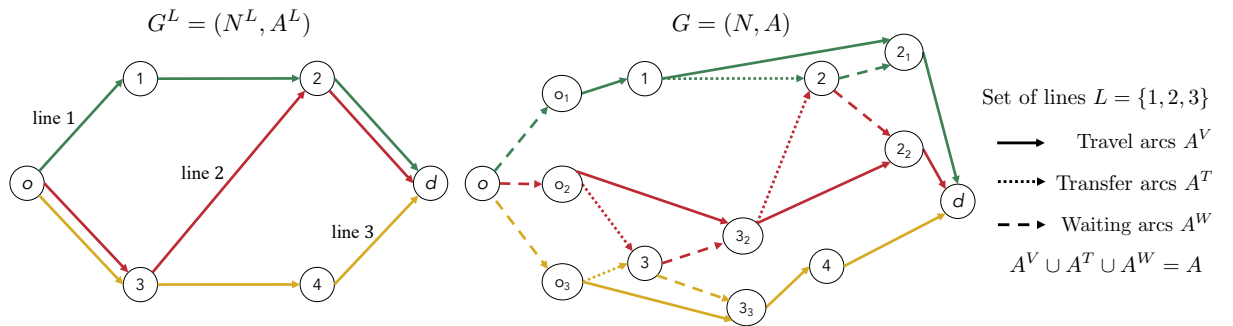


Figure 5: Modeling approach of Cervantes-Sanmiguel et al. (2023) for the transit assignment problem in the lower level of our ODME problems.

Figure 6(a) exhibits passengers travelling from origin o to destination d with the following route: first, they board Line 1 and travel from the origin o to stop 2; then, they transfer to Line 2 and continue their journey from stop 2 to the destination d . This route can be represented in network G with the sequence of nodes $o - o_1 - 1 - 2 - 2_2 - d$ (see Figure 6(b)), where arc (o, o_1) represents the passengers' waiting action at the origin before boarding Line 1. Then, from $(o_1, 1)$, passengers travel on Line 1's vehicle. Next, from $(1, 2)$, they continue on Line 1's vehicle but need to alight at stop 2 to transfer to Line 2. At that point, they need to wait again, which is reflected in the arc $(2, 2_2)$, and finally, they continue their journey from $(2_2, d)$ to reach their destination d . Note that all routes can be represented in network G ; thus, the passenger assignment problem can be solved by a minimum cost flow problem in the extended network with specific capacity constraints (due to vehicle capacities and lines' frequencies), and the optimal solution represents the minimum total travel time in the network. We highlight that outdated flows are also generated with this model using the outdated demand as input. We highlight that different assignment models could be used to define other optimisation problems, but we use our proposed approach since it also considers hard constraints of capacity of arcs associated with transit lines, which is suitable in the context of public transport networks.

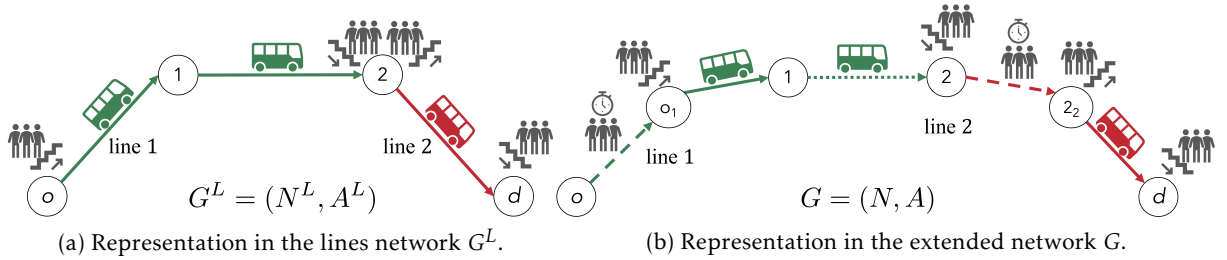


Figure 6: Representation of an example path that passengers can follow to get from the origin o to the destination d .

In the case of different types of information, we consider the following input that will lead to different models for the ODME problem.

1. The first type of information is the outdated demand. In particular, we define parameters $\hat{g}_k$ to represent passengers travelling from o_k to d_k for each OD pair $k \in K$ in the outdated demand. Note that by solving our assignment problem considering the outdated demand $\hat{g}_k$, we can obtain an outdated passenger flow denoted as $\hat{v}_a^k$ for each arc $a \in A$ and OD pair $k \in K$. The latter means that we assume passengers travel through the shortest path with available capacity, which

holds true for both when the data for the outdated matrix was collected and for the present time. We proposed using additional information to guide our model towards a more accurate estimation.

2. The structural information of the outdated demand is represented with the proportion of demand $\hat{g}_k$ for each OD pair $k = (o_k, d_k)$ among all passengers in the system, which is defined as $\hat{P}^k = \frac{\hat{g}_k}{\sum_{k \in K} \hat{g}_k}$. In the case of structural properties of the outdated passenger flow, we define $\hat{P}_a^k = \frac{\hat{v}_a^k}{\hat{g}_k}$ as the proportion of the outdated flow $\hat{v}_a^k$ of passengers travelling from o_k to d_k through arc $a \in A$ (using the associated line $l(a) \in L$) in the extended network, among all passengers $\hat{g}_k$ associated to that origin-destination pair $k \in K$.
3. The current passenger flow in lines along specific arcs of the transit network is represented as observed flow, where $\bar{A} \subseteq A^L$ is the set of arcs with observed flow $\bar{v}_{\bar{a}}$ of passengers travelling in line $l(\bar{a})$ through arc $\bar{a} \in \bar{A}$, which represents a segment of the line $l(\bar{a})$. Note that our arcs represent segments of lines and should not be confused with a roadway used by vehicles from different lines.
4. The number of passengers boarding and alighting at specific stops can also be valuable information. This information can be extracted through the analysis of ticket data and other sources. Then, we define observed stops $\bar{N} \subseteq N^L$ of the transit network G^L , where we denote with $pa x_{\bar{n}}^+$ and $pa x_{\bar{n}}^-$ the passengers boarding and alighting at stop $\bar{n} \in \bar{N}$.

Now, we introduce the following real non-negative decision variables for our models, where variables $\mathbf{v}$ of passenger flow through the different arcs in the transit network are the only ones corresponding to the lower-level problem.

- $\mathbf{g}_k$: estimated demand from origin o_k to destination d_k , for each $k \in K$.
- $\delta_k^+(\delta_k^-)$: deficit (excess) variable to measure the deviation between the estimated and outdated demand of pair $k \in K$.
- $\delta_{ka}^+(\delta_{ka}^-)$: deficit (excess) variable to measure the deviation between the estimated and outdated passenger flow through arc $a \in A$ of pair $k \in K$.
- $\delta_{\bar{a}}^+(\delta_{\bar{a}}^-)$: deficit (excess) variable to measure the deviation between the estimated and observed passenger flow through arc $\bar{a} \in \bar{A}$.
- $\gamma_k^+(\gamma_k^-)$: deficit (excess) variable to measure the deviation between the estimated and outdated matrix structure proportion of each pair $k \in K$. We highlight that the matrix structure data can be obtained from boarding and alighting information.

- $\gamma_{ka}^+(\gamma_{ka}^-)$: deficit (excess) variable to measure the deviations between the estimated and outdated flow proportion through arc $a \in A$ of pair $k \in K$.
- $\mathbf{v}_a^k$: passenger flow from origin o_k to destination d_k through the arc $a \in A$, using the associated line $l(a) \in L$.

Based on the notation above, we describe the following mathematical formulation, including all the characteristics of our ODME problems. We highlight that only some of the optional elements will be chosen regarding the kind of information assumed as an input (see Section 3.4.1 for a detailed description of our model variants). We highlight that our model is formulated using the extended network G . This means that each arc is exclusive to a single line, and we can identify waiting, transfers, and travel actions based on the different types of arcs. The only information based on the lines network G^L is the observed data $(\bar{A}$ and $\bar{N})$, which is rewritten for use within the G network in our model.

$$DirectDev(\delta) = \beta_1 \sum_{k \in K} (\delta_k^+ + \delta_k^-) + \beta_2 \sum_{k \in K} \sum_{a \in A} (\delta_{ka}^+ + \delta_{ka}^-) + \beta_3 \sum_{\bar{a} \in \bar{A}} (\delta_{\bar{a}}^+ + \delta_{\bar{a}}^-) \quad (3.1)$$

The objective function (3.1) of the upper level is the weighted sum of deviations for the following direct comparisons: (i) estimated demand compared to outdated demand, (ii) generated flows compared to outdated flows, and (iii) generated flows compared to observed flows. The goal of using the outdated information on demand and flows in the first two terms of the objective function is to guide the model during the optimisation phase to obtain a behaviour of demand and passenger flows similar to the outdated data. That said, the observed flows $\bar{v}_{\bar{a}}$ represent the current information of the system, but as stated by Lundgren and Peterson (2008), it may be impossible to generate an ODM satisfying those observed flows. Therefore, we will use soft constraints and optimise the deviation function for observed flows in the third term of (3.1).

$$StructDev(\gamma) = \beta_4 \sum_{k \in K} (\gamma_k^+ + \gamma_k^-) + \beta_5 \sum_{k \in K} \sum_{a \in A} (\gamma_{ka}^+ + \gamma_{ka}^-) \quad (3.2)$$

As stated by Behara et al. (2020), common objective functions for ODM estimation problems are based on direct comparisons concerning the ODM entries or arc flows, as in function (3.1), neglecting structural properties such as proportions of demand and flows. In response, we propose the objective function (3.2) to analyse the impact of using the information on the structural properties of outdated data, which are optional to be optimised. The first term is the deviation of the demand proportion for each OD

pair k among the total demand. In contrast, the second term is the deviation of the flow proportion of passengers travelling from each OD pair $k \in K$ through each arc a in respect to the total demand of the OD pair k . Thus, our bi-level model, including optional components (indicated within brackets), is described as follows.

$$\min \text{DirectDev}(\delta) + \left\{ \text{StructDev}(\gamma) \right\}$$

s.t.

$$\mathbf{g}_k - \delta_k^- + \delta_k^+ = \hat{g}_k \quad \forall k \in K \quad (\text{U1})$$

$$\mathbf{v}_a^k - \delta_{ka}^- + \delta_{ka}^+ = \hat{v}_a^k \quad \forall a \in A - \bigcup_{\bar{a} \in \bar{A}} \{a, t(a)\}, k \in K \quad (\text{U2})$$

$$\sum_{k \in K} (\mathbf{v}_a^k + \mathbf{v}_{t(a)}^k) - \delta_a^- + \delta_a^+ = \bar{v}_a \quad \forall \bar{a} \in \bar{A} \quad (\text{U3})$$

$$\left\{ \left(\hat{P}^k \sum_{k' \in K} \mathbf{g}_{k'} \right) - \gamma_k^- + \gamma_k^+ = \mathbf{g}_k \right\} \quad \forall k \in K \quad (\text{U4})$$

$$\left\{ \left(\hat{P}_a^k \mathbf{g}_k \right) - \gamma_{ka}^- + \gamma_{ka}^+ = \mathbf{v}_a^k \right\} \quad \forall k \in K, a \in A \quad (\text{U5})$$

$$\left\{ \sum_{k \in K: o_k = \bar{n}} \mathbf{g}_k = \text{pax}_{\bar{n}}^+ \right\} \quad \forall \bar{n} \in \bar{N} \quad (\text{U6})$$

$$\left\{ \sum_{k \in K: d_k = \bar{n}} \mathbf{g}_k = \text{pax}_{\bar{n}}^- \right\} \quad \forall \bar{n} \in \bar{N} \quad (\text{U7})$$

$$\mathbf{g}_k, \delta_k^-, \delta_k^+ \geq 0 \quad \forall k \in K \quad (\text{U8})$$

$$\delta_a^-, \delta_a^+ \geq 0 \quad \forall a \in \bar{A} \quad (\text{U9})$$

$$\delta_{ka}^-, \delta_{ka}^+, \mathbf{v}_a^k \geq 0 \quad \forall k \in K, a \in A \quad (\text{U10})$$

Where for each arc $a \in A$ and for all $k \in K$, variables $\mathbf{v}_a^k$ solve the following program.

$$\min \text{Assign}(\mathbf{v}) = \sum_{k \in K} \sum_{a \in A} c_a \mathbf{v}_a^k$$

s.t.

$$\sum_{k \in K} (\mathbf{v}_a^k + \mathbf{v}_{t(a)}^k) \leq qf_{l(a)} \quad \forall a \in A^V \quad (\text{L1})$$

$$\sum_{k \in K} \mathbf{v}_a^k \leq qf_{l(a)} \quad \forall a \in A^W \quad (\text{L2})$$

$$\sum_{a \in A_{o_k}^+} \mathbf{v}_a^k - \sum_{a \in A_{o_k}^-} \mathbf{v}_a^k = \mathbf{g}_k \quad \forall k \in K, o_k \in N \quad (\text{L3})$$

$$\sum_{a \in A_{d_k}^+} \mathbf{v}_a^k - \sum_{a \in A_{d_k}^-} \mathbf{v}_a^k = -\mathbf{g}_k \quad \forall k \in K, d_k \in N \quad (\text{L4})$$

$$\sum_{a \in A_n^+} \mathbf{v}_a^k - \sum_{a \in A_n^-} \mathbf{v}_a^k = 0 \quad \forall k \in K, n \in N - \{o_k, d_k\} \quad (\text{L5})$$

$$\mathbf{v}_a^k \geq 0 \quad \forall k \in K, a \in A \quad (\text{L6})$$

Constraints (U1)–(U3) define deviation variables δ , which are optimised in objective function (3.1). In particular, equations (U1) compute deviations between estimated and outdated demand, while constraints (U2) are for estimated and outdated flows, except arcs where demand is observed. Finally, restrictions (U3) compare the estimated flow and observed flow in both travel and transfer arcs because they represent the same physical path. Moreover, we define our optional or soft constraints for the upper level in terms of the assumed information for the optimisation problems. First, equations (U4) and (U5) compare the demand and flow proportions generated by our decision variables concerning the outdated ones and compute the deviation variables γ to be minimised in the objective function (3.2). For example, in constraint (U4), $\hat{P}^k$ is the proportion of passengers travelling from o_k to d_k regarding the total outdated demand; thus, the product between $\hat{P}^k$ and the estimated total demand $\sum_{k \in K} \mathbf{g}_k$ results in a number of passengers travelling from o_k to d_k , which should approximate the estimated demand $\mathbf{g}_k$ for OD pair $k \in K$, and similarly for equations (U5). We define constraints for given information on passenger flow at specific stops $\bar{N}$. In particular, constraints (U6) and (U7) guarantee that passengers boarding and alighting at stop $\bar{n} \in \bar{N}$ correspond to the observed passengers flow values $pac_{\bar{n}}^+$ and $pac_{\bar{n}}^-$, respectively. In contrast to the observed flows, which are precise information for which an ODM may not exist that reproduces observed flows precisely, the amount of passengers boarding and alighting at specific stops is a piece of information with less detail; therefore, we decided to include it as a hard constraint. Indeed, notice that the parameter $pac_{\bar{n}}^+$ ($pac_{\bar{n}}^-$) should match the sum of the entries for row (column) $\bar{n} \in \bar{N}$ of the ODM.

The lower level problem is described by constraints (L1)–(L6), and the objective function $Assign(\mathbf{v})$ aiming to minimise the total travel times. Constraints (L1) restrict the total passenger flow (considering all the OD pairs) along the travel arc $a \in A^V$ (associated to line $l(a)$) and the transfer arc $t(a) \in A^T$ representing the same route segment of line $l(a)$ to be within the capacity limits due to vehicle capacity q and the frequency $f_l(a)$ of line $l(a)$. The inequalities (L2) allow passenger flow through the arc $a \in A^W$, where $q \cdot f_{l(a)}$ is an upper bound of the passenger flow through arc a . The equations (L3)–(L5) are flow balance constraints for each OD pair (o_k, d_k) and node $n \in N$. The nature of the variables is defined by (U8)–(U10).

We assume an optimistic approach, i.e., we assume that when the lower-level (follower) problem has multiple optimal solutions, the follower will choose the one that is most favorable to the upper-level (leader) decision-maker (see Dempe, 2002). Note that the terms (3.1) and (3.2) in the objective function of the upper level include the variables δ_{ka} and γ_{ka} , whose values are directly defined in terms of the decision variables $\mathbf{v}_a^k$ of the lower level. Moreover, we only use real and non-negative decision variables, leading to linear bi-level programming formulations. However, even a linear bi-level program is NP-Hard, as stated by Jeroslow (1985), and there is no general-purpose solver capable of obtaining feasible solutions for it. Thus, we propose a methodological approach to reformulate the bi-level models into single-level linear formulations using Karush-Kuhn-Tucker (KKT) conditions and solve those reformulations to optimality using commercial solver, leading to near-optimal solutions of the bi-level programs (see details of standard reformulation approaches in Bard, 1998; Dempe, 2002). Since we are assuming an optimistic approach, when multiple optimal solutions exist at the lower level, the objective function in the single-level reformulation will select the configuration of lower-level variables that yields the best value for the upper-level objective function.

3.3 SOLUTION METHODOLOGY: SINGLE-LEVEL REFORMULATION

To reformulate our bi-level models into a single-level one and be able to solve it through a general-purpose solver, we can replace the lower-level problem $\{\min \text{Assign}(\mathbf{v}) : (\text{L1}) - (\text{L6})\}$ by its primal-dual optimality conditions. Initially, we must consider the upper-level variables as constants. In this case, $\mathbf{g}_k$ is treated as a parameter in the lower level. As a result, the dual problem associated with the lower level is formulated as follows.

$$\max D(\mathbf{u}) = - \sum_{a \in A^V} qf_{l(a)} \mathbf{u}_a^1 - \sum_{a \in A^W} qf_{l(a)} \mathbf{u}_a^2 + \sum_{k \in K} (\mathbf{g}_k \mathbf{u}_{o_k k}^3 - \mathbf{g}_k \mathbf{u}_{d_k k}^3) \quad (3.3)$$

s.t.

$$- \mathbf{u}_a^1 + \mathbf{u}_{i(a)k}^3 - \mathbf{u}_{j(a)k}^3 \leq c_a \quad \forall a \in A^V, k \in K \quad (\text{R1})$$

$$- \mathbf{u}_a^2 + \mathbf{u}_{i(a)k}^3 - \mathbf{u}_{j(a)k}^3 \leq c_a \quad \forall a \in A^W, k \in K \quad (\text{R2})$$

$$- \mathbf{u}_{v(a)}^1 + \mathbf{u}_{i(a)k}^3 - \mathbf{u}_{j(a)k}^3 \leq c_a \quad \forall a \in A^T, k \in K \quad (\text{R3})$$

$$\mathbf{u}_a^1, \mathbf{u}_a^2 \geq 0 \quad \forall a \in A^V, a \in A^W \quad (\text{R4})$$

$$\mathbf{u}_{nk}^3 \in \mathbb{R} \quad \forall n \in N, k \in K \quad (\text{R5})$$

Where $\mathbf{u}_a^1$, $\mathbf{u}_a^2$, and $\mathbf{u}_{nk}^3$ are dual variables associated with constraints (L1), (L2), and (L3)–(L5) of the lower-level problem, respectively. The notations $i(a)$ and $j(a)$ are the start and end nodes of arc $a \in A$, respectively. Meanwhile, $v(a) \in A^V$ represents the same travel trajectory as arc $a \in A^T$, but without transfer to another line. Notice that our objective function (3.3) has three terms associated with the right side of each family of constraints (L1)–(L5). Moreover, the objective function $Assign(\mathbf{v})$ in the lower level is defined in terms of the cost and flow for all arcs $a \in A$ and OD pair $k \in K$, while the constraints have flow variables with coefficients $\{1, -1\}$ in the left side; thus, to define all the constraints in the dual problem, we create a constraint for each pair (a, k) with $a \in A^V \cup A^W \cup A^T$ and $k \in K$ with right side c_a , where we only need to identify which constraints in the lower level include the flow variable v_a or $-v_a$ to add the associated dual variables $\mathbf{u}$ in the left side.

Thus, we will use the following constraints to represent optimality for the lower-level problem of the **ODME**.

$$\sum_{k \in K} \sum_{a \in A} c_a \mathbf{v}_a^k = - \sum_{a \in A^V} q_{fl(a)} \mathbf{u}_a^1 - \sum_{a \in A^W} q_{fl(a)} \mathbf{u}_a^2 + \sum_{k \in K} (\mathbf{g}_k \mathbf{u}_{o_k k}^3 - \mathbf{g}_k \mathbf{u}_{d_k k}^3) \quad (\text{R4})$$

It is important to observe that the right-hand side of equation (R4) is not linear due to products of variables $\mathbf{g}$ and $\mathbf{u}^3$. To linearise, we implement the McCormick envelop relaxation approach, which is a relaxation technique well-suited for addressing a group of non-linear problems including products of two real variables (MirHassani and Hooshmand, 2019), as $\mathbf{g}_k \mathbf{u}_{o_k k}^3$ and $\mathbf{g}_k \mathbf{u}_{d_k k}^3$.

Considering that $0 \leq \mathbf{g}_k \leq g^U$ and $0 \leq \mathbf{u}_{nk}^3 \leq u^U$, and making the variable substitution $x_k = \mathbf{g}_k \mathbf{u}_{o_k k}^3$, $\forall k \in K$ we add the following constraints.

$$x_k \geq g^U \mathbf{u}_{o_k k}^3 + \mathbf{g}_k u^U - g^U u^U \quad \forall k \in K \quad (\text{R5})$$

$$x_k \leq \mathbf{g}_k u^U \quad \forall k \in K \quad (\text{R6})$$

$$x_k \leq g^U \mathbf{u}_{o_k k}^3 \quad \forall k \in K \quad (\text{R7})$$

Analogously, $y_k = \mathbf{g}_k \mathbf{u}_{d_k k}^3$, $\forall k \in K$ we add the following constraints.

$$y_k \geq g^U \mathbf{u}_{d_k k}^3 + \mathbf{g}_k u^U - g^U u^U \quad \forall k \in K \quad (\text{R8})$$

$$y_k \leq \mathbf{g}_k u^U \quad \forall k \in K \quad (\text{R9})$$

$$y_k \leq g^U \mathbf{u}_{d_k k}^3 \quad \forall k \in K \quad (\text{R10})$$

It is essential to highlight that this approach requires identifying lower and upper bounds for each variables $\mathbf{g}$ and $\mathbf{u}^3$, which can be determined based on the problem's structure and considering other constraints. In our case, g_k represents demand for a single OD pair k ; thus g^U could be the total demand. In the case of variables u_{nk}^3 , according to Spiess and Florian (1989), these dual variables are related to the total travel time from node $n \in N$ to the destination node d_k ; thus, u^U could be the total travel time using all arcs $a \in A$. However, it should be highlighted that proving that the given bounds do not cut off any optimal point of the lower-level problem is as difficult as solving the bi-level problem itself (Kleinert et al., 2020).

Based on the above, the following linear program represents the reformulations of our bi-level programs.

$$\begin{aligned}
 \min \quad & DirectDev(\delta) + \left\{ StructDev(\gamma) \right\} \\
 \text{s.t.} \quad & \\
 & \mathbf{g}_k - \delta_k^- + \delta_k^+ = \hat{g}_k \quad \forall k \in K \quad (\text{U1}) \\
 & \mathbf{v}_a^k - \delta_{ka}^- + \delta_{ka}^+ = \hat{v}_a^k \quad \forall a \in A - \bigcup_{\bar{a} \in \bar{A}} \{a, t(a)\}, k \in K \quad (\text{U2}) \\
 & \sum_{k \in K} (\mathbf{v}_a^k + \mathbf{v}_{t(a)}^k) - \delta_a^- + \delta_a^+ = \bar{v}_{\bar{a}} \quad \forall \bar{a} \in \bar{A} \quad (\text{U3}) \\
 & \left\{ \left(\hat{P}^k \sum_{k' \in K} \mathbf{g}_{k'} \right) - \gamma_k^- + \gamma_k^+ = \mathbf{g}_k \right\} \quad \forall k \in K \quad (\text{U4}) \\
 & \left\{ \left(\hat{P}_a^k \mathbf{g}_k \right) - \gamma_{ka}^- + \gamma_{ka}^+ = \mathbf{v}_a^k \right\} \quad \forall k \in K, a \in A \quad (\text{U5}) \\
 & \left\{ \sum_{k \in K: o_k = \bar{n}} \mathbf{g}_k = pa x_{\bar{n}}^+ \right\} \quad \forall \bar{n} \in \bar{N} \quad (\text{U6}) \\
 & \left\{ \sum_{k \in K: d_k = \bar{n}} \mathbf{g}_k = pa x_{\bar{n}}^- \right\} \quad \forall \bar{n} \in \bar{N} \quad (\text{U7}) \\
 & \sum_{k \in K} (\mathbf{v}_a^k + \mathbf{v}_{t(a)}^k) \leq qf_{l(a)} \quad \forall a \in A^V \quad (\text{L1}) \\
 & \sum_{k \in K} \mathbf{v}_a^k \leq qf_{l(a)} \quad \forall a \in A^W \quad (\text{L2}) \\
 & \sum_{a \in A_{o_k}^+} \mathbf{v}_a^k - \sum_{a \in A_{o_k}^-} \mathbf{v}_a^k = \mathbf{g}_k \quad \forall k \in K, o_k \in N \quad (\text{L3}) \\
 & \sum_{a \in A_{d_k}^+} \mathbf{v}_a^k - \sum_{a \in A_{d_k}^-} \mathbf{v}_a^k = -\mathbf{g}_k \quad \forall k \in K, d_k \in N \quad (\text{L4})
 \end{aligned}$$

$$\sum_{a \in A_n^+} \mathbf{v}_a^k - \sum_{a \in A_n^-} \mathbf{v}_a^k = 0 \quad \forall k \in K, n \in N - \{o_k, d_k\} \quad (\text{L5})$$

$$-\mathbf{u}_a^1 + \mathbf{u}_{i(a)k}^3 - \mathbf{u}_{j(a)k}^3 \leq c_a \quad \forall a \in A^V, k \in K \quad (\text{R1})$$

$$-\mathbf{u}_a^2 + \mathbf{u}_{i(a)k}^3 - \mathbf{u}_{j(a)k}^3 \leq c_a \quad \forall a \in A^W, k \in K \quad (\text{R2})$$

$$-\mathbf{u}_{v(a)}^1 + \mathbf{u}_{i(a)k}^3 - \mathbf{u}_{j(a)k}^3 \leq c_a \quad \forall a \in A^T, k \in K \quad (\text{R3})$$

$$\begin{aligned} \sum_{k \in K} \sum_{a \in A} c_a \mathbf{v}_a^k = & - \sum_{a \in A^V} qf_{l(a)} \mathbf{u}_a^1 \\ & - \sum_{a \in A^W} qf_{l(a)} \mathbf{u}_a^2 + \sum_{k \in K} (x_k - y_k) \end{aligned} \quad (\text{R4})$$

$$x_k \geq g^U \mathbf{u}_{o_k}^3 + \mathbf{g}_k u^U - g^U u^U \quad \forall k \in K \quad (\text{R5})$$

$$x_k \leq \mathbf{g}_k u^U \quad \forall k \in K \quad (\text{R6})$$

$$x_k \leq g^U \mathbf{u}_{o_k}^3 \quad \forall k \in K \quad (\text{R7})$$

$$y_k \geq g^U \mathbf{u}_{d_k}^3 + \mathbf{g}_k u^U - g^U u^U \quad \forall k \in K \quad (\text{R8})$$

$$y_k \leq \mathbf{g}_k u^U \quad \forall k \in K \quad (\text{R9})$$

$$y_k \leq g^U \mathbf{u}_{d_k}^3 \quad \forall k \in K \quad (\text{R10})$$

$$\mathbf{g}_k, \delta_k^-, \delta_k^+ \geq 0 \quad \forall k \in K \quad (\text{U8})$$

$$\delta_a^-, \delta_a^+ \geq 0 \quad \forall a \in \bar{A} \quad (\text{U9})$$

$$\delta_{ka}^-, \delta_{ka}^+, \mathbf{v}_a^k \geq 0 \quad \forall k \in K, a \in A \quad (\text{U10})$$

$$\mathbf{v}_a^k \geq 0 \quad \forall k \in K, a \in A \quad (\text{L6})$$

$$\mathbf{u}_a^1, \mathbf{u}_a^2 \geq 0 \quad \forall a \in A^V, a \in A^W \quad (\text{R11})$$

$$\mathbf{u}_{nk}^3 \in \mathbb{R} \quad \forall n \in N, k \in K \quad (\text{R12})$$

Note that constraints (R4) are redefined by using the variables x_k and y_k to linearise our models. Moreover, we recall that we use brackets for optional components of our formulations. As can be seen in the next section of our experimental stage, we are now able to solve our optimisation models using commercial solvers.

3.4 EXPERIMENTAL RESULTS

This section provides an in-depth account of the tested models and instance generation process and presents the numerical results. We detail how each type of information impacts the accuracy of ODM estimation within each model (similarly to Ait-Ali and Eliasson, 2022).

3.4.1 MODEL VARIANTS FOR THE ODME PROBLEM

In this section, we use different ODME models based on the different types of information that can be considered as input in the decision process. We aim to identify what kind of data and amount of it has the most significant impact on ODM estimation. This analysis allows us to simplify our optimisation models by incorporating only essential constraints and objective function terms while potentially enhancing computational efficiency. By removing non-essential data, we mitigate the risk of the model over-fitting to noise or irrelevant data, which could adversely affect its estimation capability. Additionally, avoiding collecting irrelevant information leads to the decision maker's more efficient resource utilisation, dedicating time and effort exclusively towards areas that genuinely impact the model's performance.

Table 2 shows the tested models. The first column is the model name, while the second and third columns exhibit the presence of optional constraints for structural properties and boarding/alighting passengers, respectively. We recall that all of our models include constraints (U1)–(U3), (L1) – (L5), and (R1) – (R10). Finally, the last column indicates the objective function to be optimised.

Model	Soft constraints of structural properties (U4), (U5)	Hard constraints of boarding/alighting (U6),(U7)	Objective function
A	×	×	$DirectDev(\delta)$
B	✓	×	$DirectDev(\delta) + StructDev(\gamma)$
C	×	✓	$DirectDev(\delta)$
D	✓	✓	$DirectDev(\delta) + StructDev(\gamma)$

Table 2: Variant models for our ODME problem based on the different type of information assumed as input in the decision-making.

We highlight that constraints (U1), (U2), and (U3), associated with data of outdated and observed flows, are included in all of our models, since preliminary experiments show improved performance when using them. We implemented these models using the commercial solver CPLEX 22.1, employing Concert Technology in C++. We carried out the implementation on a Mac Pro with a 3.5 GHz Intel Xeon E5 processor featuring six cores and 16 GB of RAM.

3.4.2 GENERATED INSTANCES BASED ON MANDL'S NETWORK

To test the variety of models, we generated scenarios using a solution from Cervantes-Sanmiguel et al. (2023) for the benchmark Mandl's Swiss network (Mandl, 1980). Figure

Stops	0	1	2	3	4	5	6	7	8	9	10	11	12	13	14
0	0	400	200	60	80	150	75	75	30	160	30	25	35	0	0
1	400	0	50	120	20	180	90	90	15	130	20	10	10	5	0
2	200	50	0	40	60	180	90	90	15	45	20	10	10	5	0
3	60	120	40	0	50	100	50	50	15	240	40	25	10	5	0
4	80	20	60	50	0	50	25	25	10	120	20	15	5	0	0
5	150	180	180	100	50	0	100	100	30	880	60	15	15	10	0
6	75	90	90	50	25	100	0	50	15	440	35	10	10	5	0
7	75	90	90	50	25	100	50	0	15	440	35	10	10	5	0
8	30	15	15	15	10	30	15	15	0	140	20	5	0	0	0
9	160	130	45	240	120	880	440	440	140	0	600	250	500	200	0
10	30	20	20	40	20	60	35	35	20	600	0	75	95	15	0
11	25	10	10	25	15	15	10	10	5	250	75	0	70	0	0
12	35	10	10	10	5	15	10	10	0	500	95	70	0	45	0
13	0	5	5	5	0	10	5	5	0	200	15	0	45	0	0
14	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0

Table 3: Outdated ODM $\hat{g}$ (trips/24 hours).

Using this as a starting point, we defined a set of 90 randomly generated instances divided into three types of change. In these instances, specific entries of $\hat{g}$ were: 1) increased, 2) decreased, and 3) both increased and decreased to generate the exact ODM $\bar{g}$. We performed the latter to simulate different demand behaviours over time from the last outdated matrix to the estimated one. We applied the variations within a $[-2\%, 5\%]$ range, taking cues from the fluctuations in the Swiss population between 1860 and 2021 (Swiss Confederation, 2022). Table 4 shows details of the generated instances. The first column presents the Instance Class in terms of how the entries of the outdated ODM varied, that is, whether they 1) increased, 2) decreased, or 3) both, as indicated in the second column, and the corresponding percentage of modified entries in the ODM, indicated in the third column. Finally, the fourth column shows the range variation of each entry; a random number within this range indicates the variation experienced by the ODM entry over time. We generated ten instances for each instance class.

Instance Class	Change	Modified Entries %	Variation Interval
<i>Incr_100%</i>	Increase	100%	(0%, 5%]
<i>Incr_75%</i>	Increase	75%	(0%, 5%]
<i>Incr_50%</i>	Increase	50%	(0%, 5%]
<i>Decr_100%</i>	Decrease	100%	[-2%, 0%)
<i>Decr_75%</i>	Decrease	75%	[-2%, 0%)
<i>Decr_50%</i>	Decrease	50%	[-2%, 0%)
<i>Both_100%</i>	Both	100%	[-2%, 5%]
<i>Both_75%</i>	Both	75%	[-2%, 5%]
<i>Both_50%</i>	Both	50%	[-2%, 5%]

Table 4: Details of the randomly generated exact ODM $\bar{g}$ for the instances.

To assess the accuracy of estimations made by each of the models, we calculated the root mean squared error (RMSE) between the exact demand $\bar{g}$ and the estimated demand $\mathbf{g}$, as well as the error between the exact demand $\bar{g}$ and the outdated demand $\hat{g}$. Subsequently, we determined the relative improvement, computed as $\left(\frac{\text{RMSE}(\bar{g}, \hat{g}) - \text{RMSE}(\bar{g}, \mathbf{g})}{\text{RMSE}(\bar{g}, \hat{g})}\right) 100\%$, to measure the difference between our estimated matrix $\mathbf{g}$ and the exact matrix $\bar{g}$. Notice that a value of 100% indicates that $\text{RMSE}(\bar{g}, \mathbf{g}) = 0$, leading to the best estimation $\mathbf{g} = \bar{g}$.

We highlight that our optimisation models optimise different indicators as a guide to estimate the OD Matrix since the exact demand is unknown; thus, the proposed relative improvement focuses only on the accuracy of the estimation and not on the terms in the objective functions. Indeed, there may be a conflict between optimising each term in the objective function individually. However, we propose a weighted objective approach because we use various types of information solely to guide the estimation of an ODM, and we select the weights based on preliminary experimentation for the instances considered in our experimental section. In particular, we solve small instances using weights within set $\{1, 30, 100\}$ for each β parameter, where the best average solutions were obtained using $\beta_1 = 1, \beta_2 = 30, \beta_3 = 100, \beta_4 = 1, \beta_5 = 30$. Notice that β_2 and β_5 are related to outdated flows and their proportions, and β_1 and β_4 to the outdated matrix and its proportions, whereas β_3 relates to observed flows.

3.4.3 LEVELS OF OBSERVED INFORMATION

There is a significant issue regarding the collection of observed information, especially within the context of transportation and public transit systems. The reliability of data gathered through sensors and cameras used for passenger counting is fundamental for accurate analysis and decision-making. While sensors and cameras can be used to count individuals, their deployment may not be consistent across all segments of lines. These devices may occasionally malfunction, leading to incomplete data collection for certain

segments. To ensure a reliable count for each segment, it is necessary for all transit vehicles operating on each line to report the number of passengers accurately. Any device failure during the journey could result in gaps in the collected information. Additionally, personnel must manually collect data in regions with limited access to advanced technologies. However, this method imposes constraints on data gathering due to its reliance on available personnel. This variability underscores the challenges in obtaining comprehensive data. Nevertheless, our experimental section addresses these considerations by examining scenarios with both complete and limited information.

The first stage of our experimental results consists of adjusting the amount of observed information. For each instance, we varied the number $|\bar{A}|$ of observed arc flows in the transit network within the set $\left\{|A^L|, \frac{|A^L|}{2}, \frac{|A^L|}{4}\right\}$, and analogously for the number of observed stops $|\bar{N}|$ to be within $\left\{|N^L|, \frac{|N^L|}{2}, \frac{|N^L|}{4}\right\}$. The information we consider as observed in our instances was obtained by solving the assignment problem (the lower level of our model) using the matrix $\bar{g}$ in the network to identify the flow of the observed arcs. For the observed stops, we calculate the boarding data by summing the elements of each row of the matrix $\bar{g}$, and the alighting data at the stops by summing the elements of each column. Therefore, the observed information is consistent with the exact matrix. We randomly chose the elements of $|\bar{A}|$ and $|\bar{N}|$ from A^L and N^L , respectively; thus, we try nine different combinations of the amount of information for each one of the 90 randomly generated instances (a total of 810 runs for each model). The above allows us to find the amount of information that provides the most accurate estimations of ODM. Counter-intuitively, the solutions for each model do not necessarily improve when considering a larger amount of observed data. This is illustrated in Figure 8, which presents the average results for each Instance Class of Model C and D in our study. In this figure, we analyse the results varying the quantity of observed flows while maintaining $|\bar{N}| = |N^L|$, i.e., all stops are observed for boarding and alighting passengers.

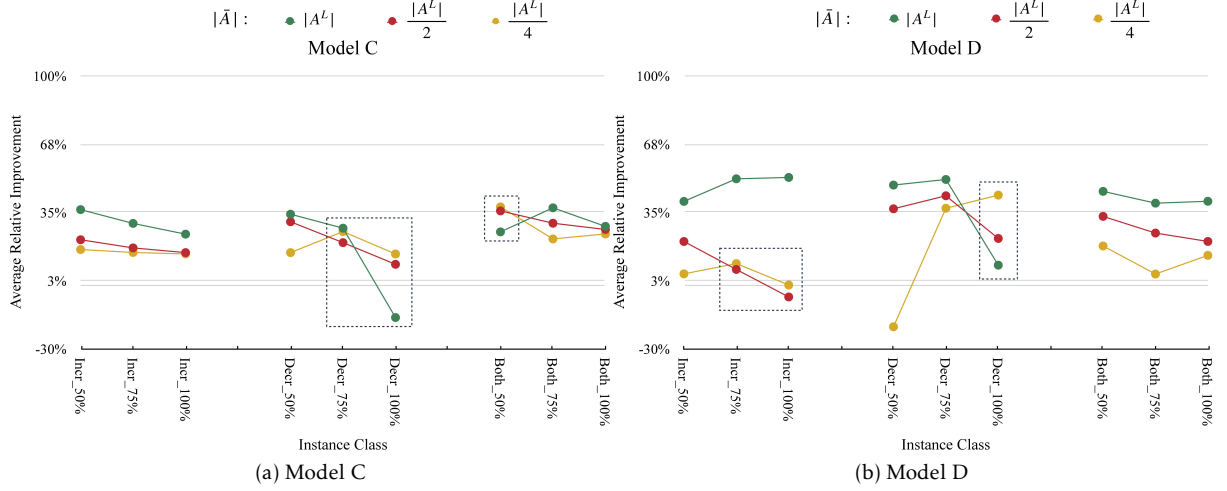


Figure 8: Performance of models varying the size of $|\bar{A}|$ and considering $|\tilde{N}| = |N^L|$.

It is important to note that in six out of the nine cases, an increased percentage of observed flows leads to an enhancement in the estimation accuracy. However, this behaviour does not hold for instances *Decr_75%*, *Decr_100%*, and *Both_50%*, where the most accurate results are achieved when only a quarter of the arcs A^L are observed (see the dotted box in Figure 8 (a)). Analogously, the same holds using Model D in instances *Decr_100%*, and for *Incr_75%* and *Incr_100%*, observing that only a quarter of A^L is better than a half of A^L (see the dotted box in Figure 8 (b)).

In particular, in the cases of models A, C, and D, the best alternative is to consider $|\bar{A}| = |A^L|$ and $|\tilde{N}| = |N^L|$ (that is, making observations at all the line segments and all the stops). However, in the case of Model B, the most accurate results are obtained by incorporating only $|\bar{A}| = \frac{|A^L|}{4}$ and $|\tilde{N}| = |N^L|$. In general, performing an exhaustive data collection for all information types is unnecessary. Indeed, the optimisation model acts as a guide to generate an ODM based on outdated and observed information about the transit network. Further qualitative analysis can be oriented to identify which arcs and stop observations have the most significant impact on the solution quality.

3.4.4 COMPARISON OF MODELS

Once we determined the best level of information (amount of data used for each data type leading to best results), for our proposed models, we compared them to find the best model on average for each instance class. In particular, Figure 9 shows the average relative improvement, where we note that the model D presents the best performance (curves of model D are the nearest ones to 100%).

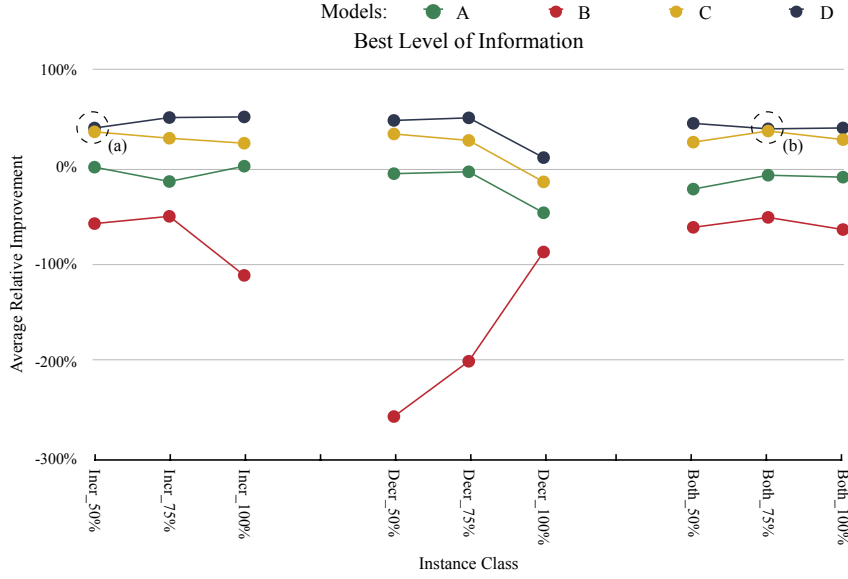


Figure 9: Performance using the best level of information for each model.

Besides identifying the model with the best average results, it is possible to evaluate the effects of using the different data types by a pair of models. In particular, we defined the indicator *dist* as the distance from the average relative improvement of the RMSE to the optimal value of 100%. Then, we computed the relative improvement $\frac{dist(\text{ModelWithoutInformationType}) - dist(\text{ModelWithInformationType})}{dist(\text{ModelWithoutInformationType})}$ of using a specific information type compared to the model without it. First, notice that if we add information on passengers boarding and alighting to models A and B, we obtain models C and D, respectively. In this scenario, the results of Model C lead to an improvement of 33.93% over Model A (see yellow and green curves in Figure 9), and the results of Model D demonstrate a 68.5% improvement over Model B (see blue and red curves in Figure 9).

Next, we compared Model A with Model B and Model C with Model D to analyse the impact of using soft constraints of structural properties and hard constraints of boarding/alighting data. Notably, the results from Model B (red curve in Figure 9) using structural properties and count passengers were, on average, 85.48% worse than those from Model A (green curve in Figure 9). Conversely, using Model D (blue curve in Figure 9) improves 21.41% on average compared to Model C (yellow curve in Figure 9). However, please note that the averages appear to be very close within the pair of points enclosed by the dashed circles, labelled as (a) and (b) in Figure 9. In point (a), for instances *Incr_50%*, Model C has an average of 36.15%, while Model D has an average of 40.07%. For point (b) with instances *Both_75%*, Model C has an average of 37%, while Model D has an average of 39.23%.

For a more detailed comparison of models C and D, Figure 10 displays the results obtained for both models for all instances of the *Incr_50%* and *Both_75%* classes (the ones with similar values of the average relative improvement).

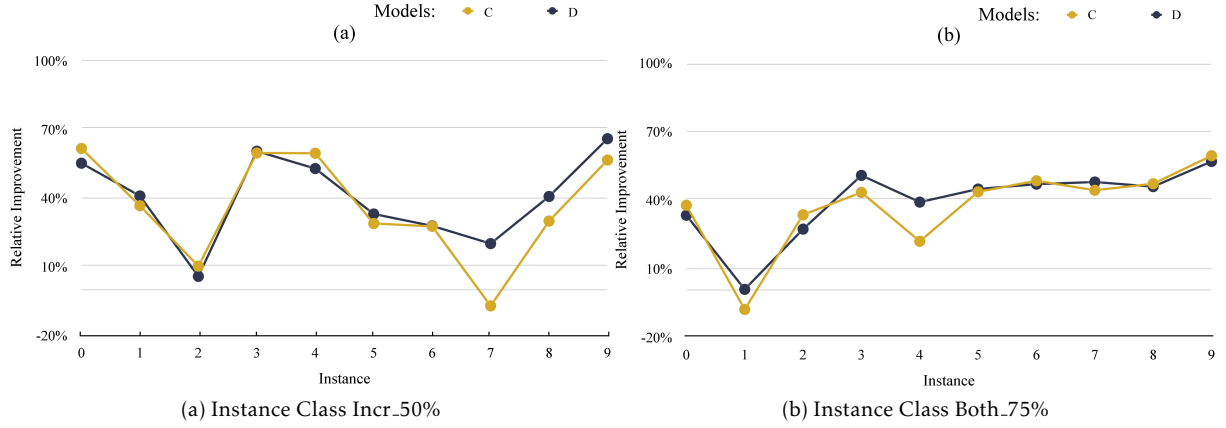


Figure 10: Results for models C and D for each instance.

We observe a very similar behaviour between the two models in both plots. In Figure 10 (a), we can see that only instances 7, 8, and 9 exhibit a more significant difference in the obtained solutions where Model C is worse than Model D. Analogously, in Figure 10 (b), we note that only instances 1, 3, and 4 show a more significant discrepancy. In the rest of the instances, both models show similar performance, which suggests that models C and D have similar behaviour. However, there are specific cases where one outperforms the other regarding obtained solutions.

Our numerical results show that it is possible to identify the effect of the different types of information to estimate an ODM through deterministic bi-level optimisation models. Finally, we recall that combining data from multiple sources may lead to inconsistency in the estimation, i.e., even considering a 100% level for a specific type of information is not enough to guarantee high-quality solutions (see Chávez-Hernández et al., 2019; Kumar et al., 2019). In general, the inconsistency of estimation models arises because different data sources may reflect different aspects of passenger flow dynamics and may not always align perfectly, for example, leading to infeasible optimisation problems if using the 100% of different types of data in hard constraints. However, this combination is needed to guide an optimisation approach like ours.

Now, we present an analysis of computational times.

3.4.5 COMPUTATIONAL TIMES

Regarding computational times, Table 5 presents the average CPU time (in seconds) required to find an optimal solution for each model for each Instance Class, along with their respective standard deviations. Note that the maximum average time found in the table is 466.76 seconds, which is relatively short, given that ODM estimations are not conducted on a daily basis.

Instance Class	A		B		C		D	
	Time	Dev	Time	Dev	Time	Dev	Time	Dev
<i>Incr_50%</i>	31.22	7.13	58.90	18.28	74.74	20.08	69.83	14.23
<i>Incr_75%</i>	29.86	9.78	54.71	13.95	80.15	21.82	76.21	33.02
<i>Incr_100%</i>	31.36	9.02	58.31	12.22	73.98	17.10	89.42	14.86
<i>Decr_50%</i>	22.92	6.94	46.49	24.01	55.27	10.77	179.92	339.87
<i>Decr_75%</i>	23.66	6.20	74.82	60.05	60.01	8.97	62.92	27.49
<i>Decr_100%</i>	20.48	4.84	45.73	17.42	54.02	12.28	62.57	19.06
<i>Both_50%</i>	32.36	10.97	58.40	17.24	61.02	8.89	82.31	24.49
<i>Both_75%</i>	177.72	474.31	52.18	17.95	58.12	16.24	104.97	78.95
<i>Both_100%</i>	466.76	1392.60	54.02	10.12	73.33	20.70	91.07	30.57

Table 5: Average computational times and their standard deviation.

Note that we achieve optimal solutions; this is possible because our optimisation approach leads us to solve linear programs as reformulations of bi-level programs, for which good quality solutions can typically be obtained in reasonable computation times. It is worth mentioning that including other additional assumptions and discrete decision variables may alter this structure of the proposed models and lead to more intractable problems.

Figure 16 shows the average CPU times from Table 5. It is worth noting that most models achieve optimality in less than 120 seconds. In cases where the average time is longer, the standard deviation also indicates a greater variability, which is caused by some atypical behaviour of the computational time. In the case of Model D on the instance class *Decr_50%*, only one instance was solved in 1146 seconds, while the others were resolved on average in 72.57 seconds, leading to a standard deviation of 18.02. As for Model A and the instance classes *Both_75%* and *Both_100%*, one instance in each class was resolved in 1,527 secs and 4,430 secs, respectively. In contrast, the remaining instances in the *Both_75%* class were resolved on average in 27.75 seconds, with a standard deviation of 7.19. In the case of the *Both_100%* class, the average resolution time was 26.38 seconds, with a standard deviation of 3.68. Hence, the average results in these points were elevated due to these outlier cases.

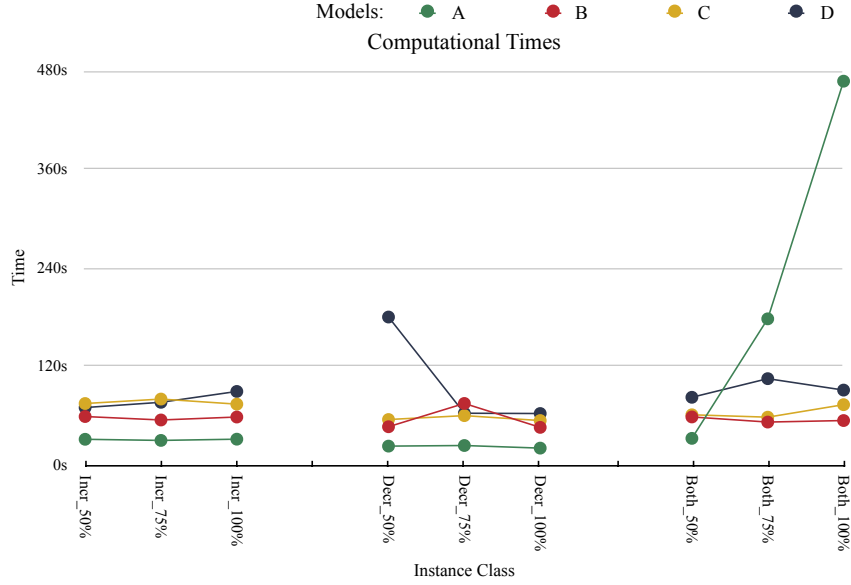


Figure 11: Computational times of solving our proposed models using a commercial optimisation solver.

In conclusion, when we exclude the outlier cases, we can discern a connection between the accuracy of the model estimations and the computational time. For instance, models C and D give better estimations than models A and B, but they require more time for their resolution.

3.5 CHAPTER SUMMARY AND REMARKS

The findings of this chapter demonstrate that the inclusion of diverse data sources significantly enhances the accuracy of origin-destination matrix estimation. In particular, the integration of boarding and alighting data proved to be especially beneficial, while relying solely on outdated ODM structures and limited flow observations resulted in reduced precision. These results emphasise the need for careful selection and combination of data in ODM estimation frameworks. The proposed models and methodological insights contribute to advancing the understanding of how data availability and structure influence public transport modelling, providing a solid foundation for future research and practical applications in network optimisation and planning. The main conclusions and future research directions derived from this study are discussed in Section 5.1 of this thesis.

CHAPTER 4

MULTI-OBJECTIVE OPTIMISATION MODEL FOR SUSTAINABLE PLANNING OF BUS FLEET REPLACEMENT

The global shift towards sustainable urban mobility requires strategic and data-driven planning to transition from diesel-based fleets to cleaner alternatives. Urban bus systems, as major contributors to emissions and noise pollution, play a crucial role in this transition. This chapter introduces a multi-objective optimisation model for the sustainable planning of bus fleet replacement, addressing economic, environmental, and social dimensions simultaneously. The proposed model determines the optimal timing, quantity, and allocation of electric buses while accounting for key constraints such as budget limitations and maximum average fleet age. By applying an epsilon-constraint method to approximate the Pareto front, this study provides insights into the inherent trade-offs between cost minimisation, environmental benefits, and equity in fleet distribution across different regions within a city.

4.1 PLANNING THE TRANSITION TO ELECTRIC BUS FLEETS

Mobility of cities around the world face significant challenges due to their reliance on diesel-powered buses. These buses contribute to environmental pollution and pose serious risks to public health. As cities strive for carbon neutrality and improved air quality, there is growing interest in transitioning public transportation fleets to electric vehicles (EVs). This shift is motivated by the potential benefits of reduced greenhouse gas emissions, reduced noise pollution, and improved urban air quality (see Ribeiro and Mendes, 2022).

However, transitioning to electric buses involves complex decision-making processes. Transportation operators must address several key issues, including the timing and quant-

ity of electric vehicles to acquire, the selection of suitable technology, and the optimal allocation of these vehicles to different bus lines. In addition, several constraints must be considered, such as electrical capacity, depot space, budget limitations, and vehicle age restrictions.

Addressing these challenges requires a holistic approach that considers not only the economic viability of adopting electric buses, but also the environmental and social impacts of this transition. Reducing costs is crucial for ensuring the financial sustainability of public transportation agencies, especially as they adapt to new technologies and infrastructure demands. Equally important is the environmental benefit of electrifying the fleet, as this transition can significantly reduce urban air pollution and greenhouse gas emissions, directly contributing to healthier communities, as it is studied for scenarios in Spain (Grijalva and Lopez Martinez, 2019), Poland (Dzikuc et al., 2021) and the United States (Du and Kommalapati, 2021). Finally, ensuring an equitable distribution of electric vehicles in various city regions is essential to provide uniform benefits, such as cleaner air and quieter streets, to all residents.

In response, we propose a tri-objective optimisation model to guide the replacement of diesel buses with electric ones in a multi-period approach (see Figure 12). Our model aims to achieve three main objectives: (1) minimise the total costs associated with vehicle purchase, infrastructure, maintenance, and battery replacements; (2) optimise a measure of gradual electrification of a transit network to reduce environmental impact; and (3) promote equity in the distribution of electric vehicles across different regions in a city. In addition, we include constraints such as bus conservation, annual investments, maximum average age of the fleet, buying used vehicles, and a target for electrification to be achieved at the end of the planning period.

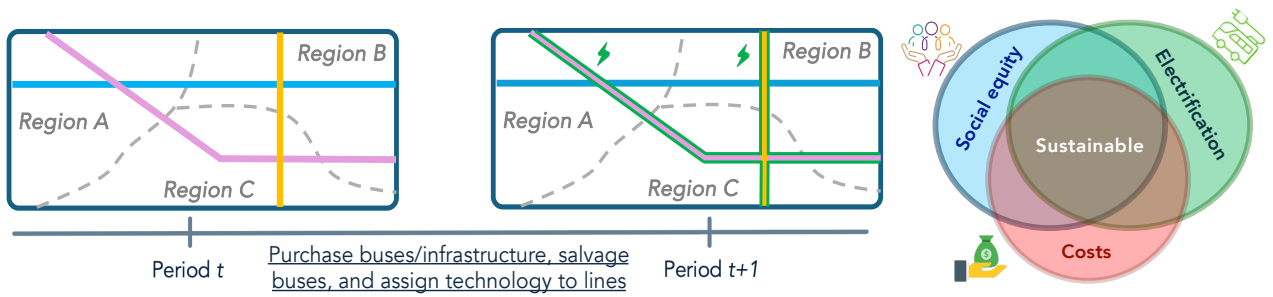


Figure 12: Scheme of our optimisation approach for the Bus Fleet Replacement Problem considering a sustainable goal.

To solve our multi-objective optimisation problem, we employ an epsilon-constraint algorithm to approximate the Pareto front, allowing us to identify a set of non-dominated

optimal solutions. Moreover, as stated by Avenali et al. (2024), a tool for evaluating some uncertainties during the planning stage is critical during the adoption of electromobility, which can be tackled with sensitivity analysis and variants of our modeling approach (as can be seen in the experimental section). In summary, our optimisation approach allows us to study the inherence of trade-offs in a sustainable philosophy, providing comprehensive new information for decision making, and leading to a valuable tool for public transportation operators and policy makers.

4.2 OPTIMISATION PROBLEM AND MATHEMATICAL FORMULATION

We recall that we are interested in planning the electrification of a transit network considering a sustainable perspective, that is, analysing social, economic, and environmental aspects of it. Then, to define our decision problem, we assume that there exists a public transport operator or government agency responsible for managing a public transport network of a city divided into multiple regions. Let L denote the set of lines in the network and R the set of regions in the city. The agency aims to gradually replace its diesel bus fleet with electric vehicles (EVs) over a multi-year planning horizon denoted by T . The bus fleet types eligible for acquisition are contained in the set B , which encompasses a variety of electric technologies and battery types ($b = 0$ is considered as diesel technology for modelling purposes). In this study, we also consider the possibility of acquiring used electric vehicles in each period $t \in T$. We define the set N to indicate the years of use of a vehicle, where 0 is considered new. Moreover, for each line $l \in L$, we assume that the length of the line in kilometres, denoted as ϕ_l , is known. Finally, for each region $r \in R$, we assume the coverage of the network km_r as given, as well as the kilometres c_{rl} covered by each transit line $l \in L$.

The goal of our optimisation problem, called Sustainable Bus Fleet Replacement **SBFR**, is to develop an electrification plan that determines decisions for each period regarding fleet renewal, the assignment of electric vehicles to specific bus lines, and the sale of buses that are no longer needed due to their age. This plan aims to optimise the objective functions of operational costs, equitable distribution of EV services between regions, and gradual electrification.

For each type of electric bus technology $b \in B$, we assume that the following parameters are given, which directly influence the long-term decision whether it is advantageous to purchase them.

- cv_{bn}^t : The purchase cost of a vehicle n years old with technology $b \in B - \{0\}$ in period $t \in T$.
- ci_b^t : The cost of purchasing infrastructure (per charger) for technology $b \in B - \{0\}$ in period $t \in T$. Where λ_{lb} chargers are needed when line $l \in L$ is operated using technology $b \in B - \{0\}$.
- cf_{bn}^t : The cost of diesel / energy for a n -year-old vehicle with technology $b \in B$ in period $t \in T$.
- cm_{bn}^t : The maintenance cost for a vehicle n years old with technology $b \in B$ in period $t \in T$.
- cb_b^t : The cost of the battery for technology $b \in B - \{0\}$ in period $t \in T$.
- $\mu_{bn} = \begin{cases} 1, & \text{if a } n\text{-year-old vehicle with technology } b \in B - \{0\} \text{ requires} \\ & \text{a battery replacement} \\ 0, & \text{otherwise} \end{cases}$
- q_{lb} : The size of the fleet of each type of technology $b \in B$ required for the line $l \in L$.

Determining the required fleet size q_{lb} for line l constitutes a complex optimisation problem, involving not only the allocation of buses but also the scheduling of trips and charging actions for each vehicle (Rogge et al., 2018). In particular, we assume that an electric vehicle must be charged to the 100% battery level after completing a trip. This assumption directly impacts the overall system, as it leads to increased cycle times for the vehicles. Consequently, a larger fleet of electric vehicles is needed to maintain the service level across all lines, compared to using vehicles that do not require charging actions.

We also include a budget P^t for each period $t \in T$, representing the available financial resources that limit the total annual cost in terms of vehicle acquisition costs cv_{bn}^t , charger installation costs ci_b^t , and ongoing operating costs, including fuel or energy (cf_{bn}^t), maintenance (cm_{bn}^t) and battery replacements (cb_b^t) that occur every τ_b consecutive years of use for vehicles with technology b . Furthermore, the budget of each period can be increased by selling vehicles that are no longer operational (the oldest vehicles with technology $b \in B$, which are at least β_b years old), with their salvage value represented by α_{bn} . We resume our notation for the input in Table 6.

Table 6: Summary of the input for our optimisation problem.

Symbol	Description
L	Set of lines in the transit network.
T	Set of planning periods.
B	Set of vehicles' technologies, i.e., the combination of battery size and the type of charging infrastructure.
N	Set of years of use for vehicles in the transit network.
R	Set of regions covered by the transit network.
cv_{bn}^t	Purchase cost of a n -year-old vehicle with technology $b \in B - \{0\}$ in period $t \in T$.
ci_b^t	Purchase cost per charger for infrastructure supporting technology $b \in B - \{0\}$ in period $t \in T$.
cf_{lb}^t	Diesel/Energy cost for each line $l \in L$ with technology $b \in B$ in period $t \in T$.
cm_{bn}^t	Maintenance cost for a n -year-old vehicle with technology $b \in B$ in period $t \in T$.
cb_b^t	Battery cost for technology $b \in B - \{0\}$ in period $t \in T$.
μ_{bn}	Binary parameter taking the value of 1 if a n -year-old vehicle with technology $b \in B - \{0\}$ requires a battery replacement (i.e., $n \bmod \tau_b = 0$), and 0 otherwise.
P^t	Budget for period $t \in T$.
q_{lb}	Fleet size with technology $b \in B$ required for line $l \in L$.
α_{bn}	Salvage value of a n -year-old vehicle of type $b \in B$.
β_b	Age of use at which a bus of type $b \in B$ can be salvaged.
γ	Maximum bus average age across all periods.
λ_{lb}	Chargers for technology $b \in B - \{0\}$ required for line $l \in L$.
km_r	Network coverage for region $r \in R$ (km).
c_{rl}	Kilometres covered in region $r \in R$ by line $l \in L$.

Our **SBFR** optimisation problem determines the allocation of technologies B to the lines L operating with conventional buses, as well as the number of electric vehicles to buy and sell for each type of technology $b \in B$ and period $t \in T$. So, we define the following decision variables.

- $y_{lb}^t = \begin{cases} 1, & \text{if line } l \in L \text{ operates with technology } b \in B - \{0\} \text{ in period } t \in T \\ 0, & \text{otherwise} \end{cases}$
- z_{bn}^t : Number of n -year-old vehicles of type $b \in B$ that are sold at the beginning of period $t \in T$
- x_{bn}^t : Number of n -year-old vehicles of type $b \in B$ that are purchased at the beginning of period $t \in T$
- v_{bn}^t : Number of n -year-old vehicles of type $b \in B$ at the beginning of period $t \in T$

- m^t : Savings of period $t \in T$

We define $(\mathbf{x}, \mathbf{y}, \mathbf{z}, \mathbf{v}, \mathbf{m})$ to represent all the decision variables. Next, we present our mixed-integer nonlinear program (MINLP) for the **SBFR** problem.

$$\min F_{COSTS}(\mathbf{x}, \mathbf{y}, \mathbf{v}) = \sum_{t \in T} \left(\sum_{b \in B - \{0\}} \sum_{n \in N} x_{bn}^t c v_{bn}^t + \sum_{l \in L} \sum_{b \in B - \{0\}} (y_{lb}^t - y_{lb}^{t-1}) c i_b^t \lambda_{lb} + \right. \\ \left. \sum_{b \in B - \{0\}} c b_b^t \sum_{n \in N} \mu_{bn} v_{bn}^t + \sum_{l \in L} \sum_{b \in B} c f_{lb}^t y_{lb}^t + \sum_{b \in B} \sum_{n \in N} c m_{bn}^t v_{bn}^t \right) \quad (4.1)$$

$$\min F_{GRADUAL}(\mathbf{y}) = \sum_{t \in T} \frac{\left(\sum_{l \in L} \sum_{b \in B - \{0\}} (y_{lb}^t - y_{lb}^{t-1}) - \frac{\sum_{t' \in T} \sum_{l' \in L} \sum_{b' \in B - \{0\}} (y_{l'b'}^{t'} - y_{l'b'}^{t'-1})}{|T|} \right)^2}{|T|} \quad (4.2)$$

$$\min F_{EQUITY}(\mathbf{y}) = \sum_{t \in T} \sum_{r \in R} \frac{\left(\sum_{l \in L} \sum_{b \in B - \{0\}} \frac{y_{lb}^t c_{rl}}{k m_r} - \frac{\sum_{r' \in R} \sum_{l' \in L} \sum_{b' \in B - \{0\}} \frac{y_{l'b'}^{t'} c_{r'l'}}{k m_{r'}}}{|R|} \right)^2}{|R|} \quad (4.3)$$

s.t.

$$v_{bn}^t = v_{bn-1}^{t-1} + x_{bn}^t - z_{bn}^t \quad \forall b \in B, t \in T, n \geq 1 \quad (4.4)$$

$$v_{b0}^t = x_{b0}^t - z_{b0}^t \quad \forall b \in B, t \in T \quad (4.5)$$

$$v_{bn}^t = 0 \quad \forall b \in B, t \in T, n \geq 14 \quad (4.6)$$

$$x_{0n}^t = 0 \quad \forall t \in T, n \geq 0 \quad (4.7)$$

$$z_{bn}^t = 0 \quad \forall b \in B, t \in T, n < \beta_b \quad (4.8)$$

$$y_{lb}^{t+1} \geq y_{lb}^t \quad \forall b \in B - \{0\}, l \in L, t \leq |T| - 1 \quad (4.9)$$

$$\sum_{l \in L} \sum_{b \in B} y_{lb}^{|T|} = |L| \quad (4.10)$$

$$\sum_{b \in B} y_{lb}^t = 1 \quad \forall l \in L, t \in T \quad (4.11)$$

$$\sum_{n \in N} v_{bn}^t = \sum_{l \in L} y_{lb}^t q_{lb} \quad \forall b \in B, t \in T \quad (4.12)$$

$$\sum_{b \in B - \{0\}} \sum_{n \in N} x_{bn}^t c v_{bn}^t + \sum_{l \in L} \sum_{b \in B - \{0\}} (y_{lb}^t - y_{lb}^{t-1}) c i_b^t \lambda_{lb}$$

$$\begin{aligned}
 & + \sum_{b \in B - \{0\}} cb_b^t \sum_{n \in N} \mu_{bn} v_{bn}^t + \sum_{b \in B} \sum_{l \in L} cf_{lb}^t y_{lb}^t \\
 & + \sum_{b \in B} \sum_{n \in N} cm_{bn}^t v_{bn}^t + m^t = \sum_{b \in B} \sum_{n \in N} z_{bn}^t \alpha_b + P^t + m^{t-1} \quad \forall t \in T \quad (4.13)
 \end{aligned}$$

$$\frac{\sum_{b \in B} \sum_{n \in N} nv_{bn}^t}{\sum_{b \in B} \sum_{n \in N} v_{bn}^t} \leq \gamma \quad \forall t \in T \quad (4.14)$$

$$x_{bn}^t, z_{bn}^t, v_{bn}^t \in \mathbb{Z}; U, m^t \in \mathbb{R}; y_{lb}^t \in \{0, 1\} \quad \forall t \in T, b \in B, n \in N, l \in L \quad (4.15)$$

The objective function (4.1) minimises the total cost associated with the purchase of electric vehicles, the charging infrastructure, the replacement of the battery, the fuel (diesel and electricity) and the maintenance of the vehicle. The objective function (4.2) minimises the variance in the increment of electrified lines of consecutive periods in T to ensure a gradual electrification of lines. Finally, the objective function (4.3) minimises the sum between all periods of variance in the fraction of electrified kilometres in all regions to ensure an equitable electrification of the city's transit network.

Regarding the constraints of the problem, equations (4.4) and (4.5) represent vehicle balance or inventory constraints. The restrictions (4.6) guarantee that there are no vehicles older than 14 years operating in the system. The constraints (4.7) ensure that conventional vehicles are not purchased. The equalities (4.8) guarantee that the vehicles have not exceeded their useful life. The constraints (4.9) ensure that if a technology $b \in B - \{0\}$ has been assigned to line $l \in L$ in period $t \in T$, that technology remains assigned to that line from that period onward. The equality (4.10) ensures that, by the end of the planning period, all lines will operate with electric vehicles. The equalities (4.11) ensure that only one technology is assigned to each line in each period. The constraints (4.12) ensure that, in each period, there are sufficient vehicles of the different technologies to meet the operation of the lines. Equalities (4.13) ensure that the budget has not been exceeded. The constraints (4.14) ensure that the average age of the vehicles in the system does not exceed the maximum allowed. Finally, the constraints (4.15) represent the nature of the variables.

4.2.1 ε -CONSTRAINT ALGORITHM FOR THE SBFR

problem Given the multi-objective nature of our **SBFR** problem, we do not prioritise identifying a single solution that optimises all objectives simultaneously. Instead, our focus is on obtaining mathematically non-dominated solutions that presents the trade-offs between the objectives. In particular, a solution vector $\mathbf{x}^*$ in the feasible space $\mathcal{X}$, is Pareto optimal for a triobjective minimisation problem, if there does not exist another

$\mathbf{x} \in \mathcal{X}$ such that $f_1(\mathbf{x}) \leq f_1(\mathbf{x}^*)$, $f_2(\mathbf{x}) \leq f_2(\mathbf{x}^*)$, $f_3(\mathbf{x}) \leq f_3(\mathbf{x}^*)$, and $f_i(\mathbf{x}) < f_i(\mathbf{x}^*)$ for some objective f_i . If $\mathbf{x}^*$ is a Pareto optimal solution, then $f(\mathbf{x}^*)$ is a non-dominated point in the objective value space (see Marler and Arora, 2004).

Then, we are looking for a good approximation of the set of non-dominated points, which is called *Pareto Front*. This approach allows the decision maker to observe the conflicts among the different objectives and to select the available options based on their criteria. In this study, we will implement the ε -constraint method, which was first introduced in Haimes (1971). This consists of optimising a single objective $f_i(\mathbf{x})$, while the other objectives are limited by additional constraints $f_j(\mathbf{x}) \leq \varepsilon_j$. Then, we can obtain an approximation of the Pareto front by varying the parameters ε_j . Figure 13 illustrates an example of the ε -constraint method applied to a bi-objective optimisation problem, where the objective function $F_1(x)$ is minimised while the second objective function is constrained by $F_2(x) \leq \varepsilon$.

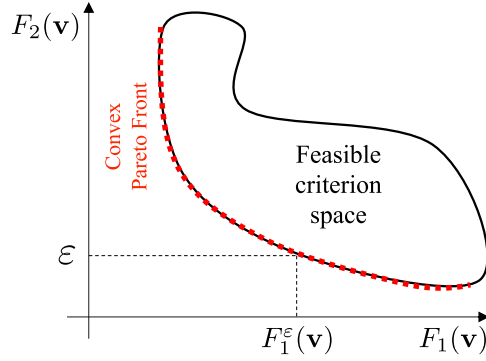


Figure 13: Example of finding non-dominated solutions using the ε -constraint algorithm.

It is widely common in Bus Fleet Replacement problems to focus on cost minimisation as the only objective function (Emiliano et al., 2020b; Pelletier et al., 2019; Islam and Lownes, 2019). Therefore, in our approach, we use F_{COSTS} as the objective function to be minimised, while $F_{GRADUAL}$ and F_{EQUITY} are incorporated as constraints, bounded by ε_G and ε_E , respectively (see details in Algorithm 1). The algorithm begins with an empty set of approximations and calculates the extreme points of the approximation (lines 1-3). These extreme points are then used to establish the range over which ε_G and ε_E will vary. We define S_{ε_G} and S_{ε_E} as the set of values to explore for ε_G and ε_E , and N_{ε_G} and N_{ε_E} as the total number of values to explore within these sets. The values within these sets range from $F_{GRADUAL}^*$ (F_{EQUITY}^*) to P_G^* (P_E^*) with an increase of Δ_{ε_G} (Δ_{ε_E}) as defined in lines 4 and 5. Based on these sets, further calculations are conducted to ensure a thorough and efficient exploration of the trade-offs between objectives.

Algorithm 1: ε -constraint for the SBFR.

Input: Instance of SBFR, N_{ε_G} , N_{ε_E}

Output: Approximation *SetPareto* of Pareto front

- 1: $SetPareto = \emptyset$
 - 2: Solve $F_{COSTS}^* = \{\min F_{COSTS}(\mathbf{x}, \mathbf{y}, \mathbf{z}) : (4.4) - (4.15)\}$,
 $P_E^* = F_{EQUITY}((\mathbf{x}, \mathbf{y}, \mathbf{z})_{COSTS}^*)$, $P_G^* = F_{GRADUAL}((\mathbf{x}, \mathbf{y}, \mathbf{z})_{COSTS}^*)$
 - 3: Solve $F_{GRADUAL}^* = \{\min F_{GRADUAL}(\mathbf{y}) : (4.4) - (4.15)\}$,
 $P_E^* = \max\{P_E^*, F_{EQUITY}(\mathbf{y}_{GRADUAL}^*)\}$
 - 4: Solve $F_{EQUITY}^* = \{\min F_{EQUITY}(\mathbf{y}) : (4.4) - (4.15)\}$,
 $P_G^* = \max\{P_G^*, F_{GRADUAL}(\mathbf{y}_{EQUITY}^*)\}$
 - 5: $\Delta_{\varepsilon_G} = \frac{P_G^* - F_{GRADUAL}^*}{N_{\varepsilon_G} - 1}$
 - 6: $\Delta_{\varepsilon_E} = \frac{P_E^* - F_{EQUITY}^*}{N_{\varepsilon_E} - 1}$
 - 7: $S_{\varepsilon_G} = \{\varepsilon_G^i \mid \varepsilon_G^i = F_{GRADUAL}^* + i\Delta_{\varepsilon_G}, i = 0, 1, \dots, N_{\varepsilon_G} - 1\}$
 - 8: $S_{\varepsilon_E} = \{\varepsilon_E^j \mid \varepsilon_E^j = F_{EQUITY}^* + j\Delta_{\varepsilon_E}, j = 0, 1, \dots, N_{\varepsilon_E} - 1\}$
 - 9: **for** $(\varepsilon_G, \varepsilon_E) \in S_{\varepsilon_G} \times S_{\varepsilon_E}$ **do**
 - 10: **Solve**
 $P_{\varepsilon_G, \varepsilon_E}^* = \{\min F_{COSTS}(\mathbf{x}, \mathbf{y}, \mathbf{v}) : (4.4) - (4.15), F_{GRADUAL} \leq \varepsilon_G, F_{EQUITY} \leq \varepsilon_E\}$
 - 11: $SetPareto = SetPareto \cup \{(P_{\varepsilon_G, \varepsilon_E}^*, F_{GRADUAL}(\mathbf{y}_{\varepsilon_G, \varepsilon_E}^*), F_{EQUITY}(\mathbf{y}_{\varepsilon_G, \varepsilon_E}^*))\}$
 - 12: **end for**
-

Finally, all experiments were performed on a MacBook Pro with an Apple M3 chip and 18GB of RAM, using CPLEX 22.1 Concert Technology, coded in C++ and using a stop criterion of 7200 seconds of computational time or a relative gap¹ of 1%. The experimental results are discussed in the next section.

x

4.3 EXPERIMENTAL RESULTS

4.3.1 NIGHTTIME PUBLIC TRANSIT SYSTEM OF SANTIAGO, CHILE

To validate our methodology on a real-world network, we examined the nighttime public transport system in Santiago, Chile. The network comprises 44 lines and serves 34 municipalities in the Metropolitan Region. We considered a 20-year planning horizon and aimed to fully electrify all routes. Seven electric bus technologies were considered for evaluation (See Table 7).

¹The relative gap is computed as $(\frac{PrimalBound - DualBound}{PrimalBound})100\%$

Type of Bus	Battery Capacity (kWh)	Price (USD) cv_{b0}^t	Battery Re- placement (USD)	Maintenance (USD)
Model 0	-	-	0	13,125.87
Model 1	385	318,304	95,491.2	3,979.24
Model 2	229	251,256	75,376.8	5,565.28
Model 3	255	257,868	77,360.4	7,910.24
Model 4	282	305,196	91,558.8	6,664.73
Model 5	326	316,448	94,934.4	4,912.95
Model 6	350	322,596	96,778.8	3,522.06
Model 7	350	334,660	100,398	5,134.32

Table 7: Technical and cost details of diesel (Model 0) and electric bus models, including battery capacity, purchase price, battery replacement cost, and annual maintenance.

The nighttime public transport network plays a vital role in ensuring mobility during non-peak hours, serving commuters across 34 municipalities in the Metropolitan Region. It provides essential connections for workers with irregular schedules, students, and others who rely on public transit at night.

Figure 14 provides a visual representation of the network, highlighting its extensive coverage and critical connections. This case study not only offers a practical application of the proposed methodology, but also contributes valuable information on the planning of sustainable and efficient public transport systems in urban areas.

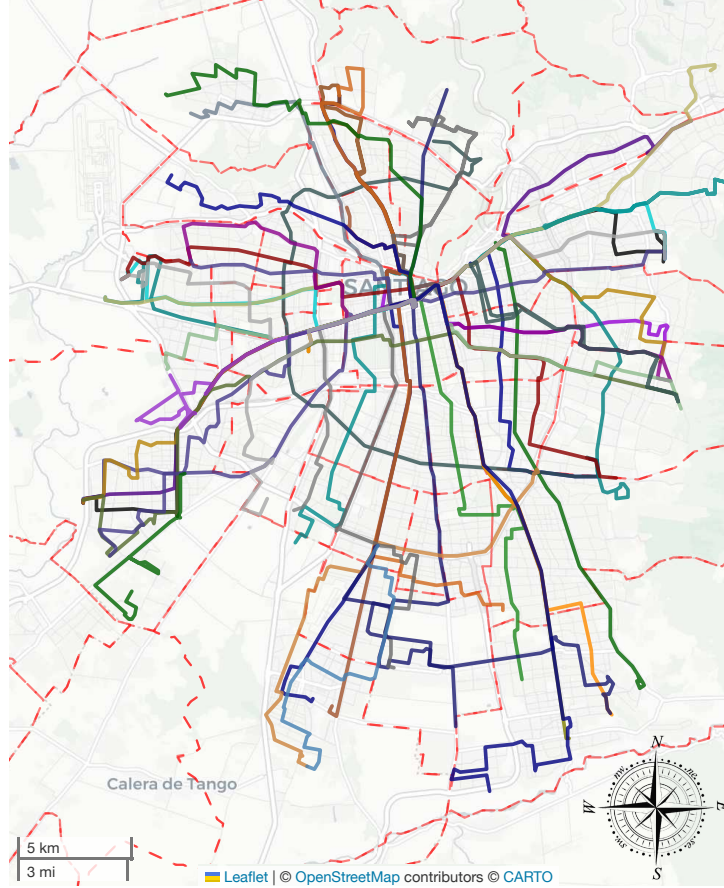


Figure 14: Nocturnal Public Transport Network of Santiago, Chile (@OpenStreetMap).

Given the growing emphasis on sustainability and environmental conservation, the transition to a fully electrified fleet over a 20-year horizon aligns with global efforts to reduce greenhouse gas emissions and dependence on fossil fuels. The electrification plan considers seven different electric bus technologies, each with different battery capacities and costs (Table 7). The evaluation focusses on selecting the optimal combination of technologies to achieve a balance between gradual electrification over time, cost-effectiveness, and equitable allocation of electric vehicles.

Two purchasing scenarios were considered. In Instance A, only new vehicles can be acquired. This restriction is modelled by setting $x_{tbn} = 0$ for all used vehicles ($n \geq 1$), all periods $t \in T$, and all bus types $b \in B$. In Instance B, both new and used vehicles can be purchased, with no restrictions on the decision variable x_{tbn} .

Table 8 summarises the assumptions used for model parameters, including purchase and depreciation costs (cv_{bn}^t), infrastructure costs (ci_b^t), annual fuel and energy costs (cf_{lb}^t), maintenance costs (cm_{bn}^t), salvage values (α_{bn}), fleet sizing (q_{lb}), and network coverage (km_r, c_{rl}). For the instances of our study, no budget restrictions were considered, repres-

ented by assigning a very high value to P^t for all t . This can be adjusted for other case studies. The minimum operational age at which a bus of type $b \in B$ (denoted β_b) becomes eligible for resale has been established at 5 years, the highest average age for buses during all periods (γ) was established at 8 years. The range of vehicle ages considered in the analysis spans $n = 0$ to 19 years. Finally, it was assumed that the number of chargers required for technology $b \in B \setminus \{0\}$ on line $l \in L$ (λ_{lb}) would be half of the fleet size q_{lb} .

Parameter	Assumption
cv_{bn}^t	For new vehicles, we considered average market prices for different technologies as it is shown in Table 7 (Kementerian Dalam Negeri Republik Indonesia, 2021). Depreciation was applied on a declining basis: 20% annually for the first 5 years, 10% for years 6 through 10, and 5% from year 11 onward.
ci_b^t	The infrastructure cost for each bus type $b \in B \setminus \{0\}$ and time $t \in T$ was assumed to be USD 68,153.8, representing the average value across available market prices (C40 Cities, 2023).
cf_{lb}^t	Annual fuel or energy cost per line l and bus type b was computed as the product of the total annual distance travelled, the corresponding energy consumption rate (diesel or electricity), and the respective unit energy cost. Diesel was priced at USD 1.02 per litre (Global Petrol Prices, 2025a) and electricity at USD 0.16 per kWh (Global Petrol Prices, 2025b). Energy prices were assumed to remain constant throughout the planning horizon. Line distances and service frequencies were derived from GTFS data (June 2024) (DTPM Chile, 2024).
cm_{bn}^t	For electric buses, maintenance costs for each bus type b at time t were randomly set between 3,500 and 8,000 USD per year, which is consistent with the maintenance costs reported for Chile in Charged Electric Vehicles Magazine (2020). For diesel buses, a fixed annual maintenance cost of 13,125.87 USD was assumed (see Table 7).
cb_b^t	Battery replacement costs account for roughly 30% of the total bus price across all models.
α_{bn}	Salvage value of bus type b of age n was assumed to be 90% of the purchasing cost cv_{bn}^0 .
q_{lb}	The fleet size for each line and bus type was estimated as the ratio of the operational cycle time to the service frequency, assuming an average speed of 40 km/h. For electric buses, charging time was included in the cycle time.
km_r, c_{rl}	Network coverage for region $r \in R$ (km) and the kilometres covered in region $r \in R$ by line $l \in L$ were derived from GEOJSON data sourced from official Chilean transport maps (Caracena, C., 2025).

Table 8: Parameter assumptions.

This structured instance, defined by the network characteristics, vehicle parameters, and operational assumptions detailed in Tables 7 and 8, serves as the input for the multi-objective optimisation model. The solution approach employs the ε -constraint algorithm, formally introduced in the following section, to identify Pareto-optimal solutions that allow us to study the trade-off between operational cost, network electrification, and equitable allocation of electric buses across the network.

4.3.2 EFFICIENCY OF THE ε -CONSTRAINT ALGORITHM

In this section, we analyse the quality of the solutions and the computational times to implement our ε -constraint method in the case study. In general, our optimisation approach is efficient since it takes less than 4 days to implement our epsilon constraint for both instances. In the case of the scenario of new vehicles, we found solutions for 57.02% of the iterations in the epsilon constraint, while in the case of purchasing new and used vehicles, we find feasible solutions for 8.09% of the iterations of our ε -constraint. Notice that since we are dealing with a multi-objective optimisation approach, the latter could happen due to the conflict between the optimisation of the two objectives bounded in the constraints during our experimental stage.

Figure 15 shows the relative gap among all iterations of our ε -constraint algorithm for both instances. The dashed lines contain the iterations corresponding to a fixed value ε_G , while the variables ε_E vary in ascending order. We also have a separator that distinguishes different values of ε_G , arranged in ascending order. Notice that we obtain smaller gaps than 1% for 94.02% of the solutions found along the iterations of our epsilon constraint when defining a plan assuming that it is possible to purchase new vehicles only, and for all iterations when purchasing new and used vehicles, that is, we obtain near-optimal solutions when implementing our solution algorithm to generate an approximation of the Pareto fronts.

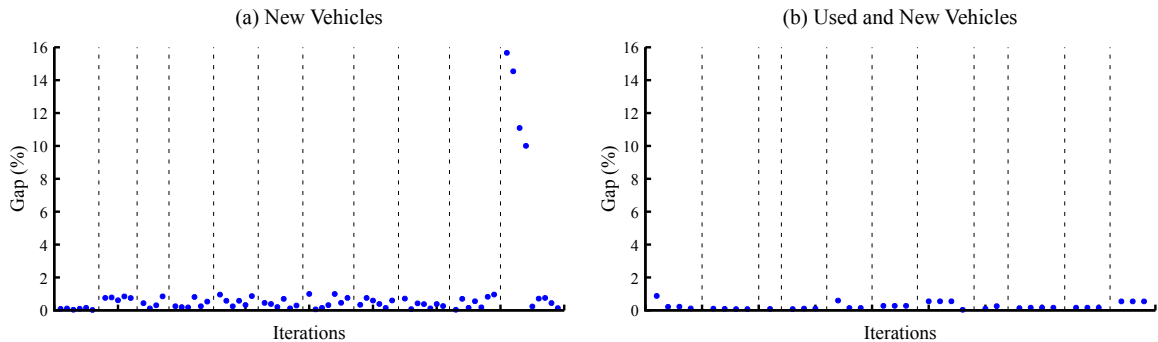


Figure 15: Relative Gaps for each iteration of the ε -constraint algorithm.

In the case of computational times, we require less than 31.4 hours to obtain solutions along the iterations of our epsilon constraint for each scenario, as shown in Figure 16. In the case of purchasing new vehicles, the longer computational times correspond to the highest value of ε_G . In the case of buying new and used vehicles, the longest computational times appear in the second value of ε_G

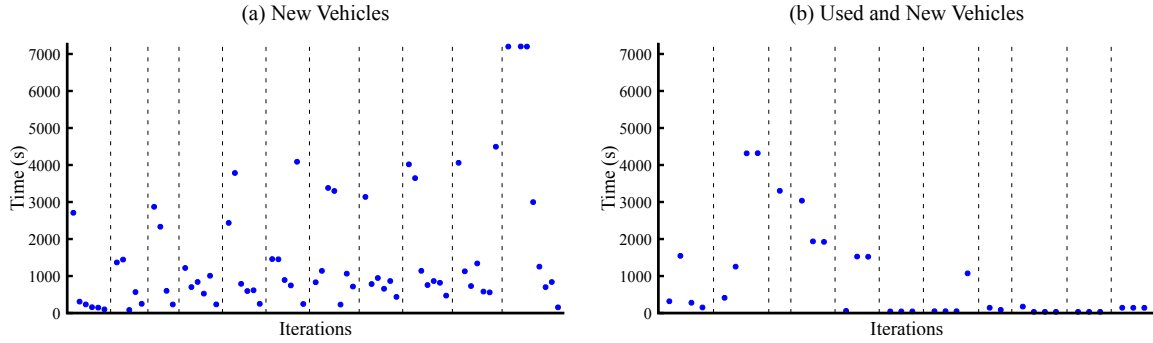


Figure 16: Computational Times for each iteration of the ε -constraint algorithm.

Summarising the analysis of the quality of the solution and the computational times of the experimental stage, our results demonstrate that the proposed multi-objective optimisation approach is effective for real-sized instances. This method supports decision making by providing new information on the trade-off involved in optimising social, economic, and ecological objectives (see the next section).

4.3.3 ANALYSING THE TRADE-OFF BETWEEN COSTS, EQUITY AND ELECTRIFICATION METRICS

In this section, we present the conflict between optimising a gradual electrification measure (ecological goal), minimising operational costs (economic goal), and optimising equity in the electrification of different areas in a region (social goal). We then address a sustainable optimisation approach with three objectives.

Figure 17 shows the Pareto front approximations obtained for the two instances, which allows only the purchase of new vehicles (left panel) and which allows the purchase of used and new buses (right panel). We can observe that there is a conflict between the optimised objectives, since there is a dispersion of points across the three axes related with the different objective functions. However, performing a visual analysis of a 3D plot to analyse the trade-off between objectives is cumbersome.

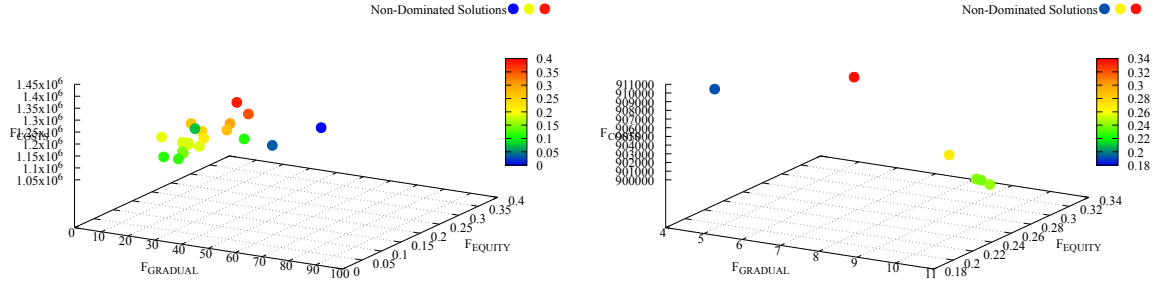


Figure 17: Pareto front approximations for instances A and B of the SBFR problem.

From now on, we will analyse the projection of the Pareto front approximation onto the Cartesian plane formed by the social and ecological objectives. In particular, we denote the cost value using a colour map that transitions from green for the lower values to red for higher values of operational costs. Figure 18 shows the projections mentioned above for both scenarios. Notice that when assuming the purchase of only new buses (see left panel), we observe that for low values of operational costs, the conflict between the social and ecological goals is more pronounced, since there are green points that form a Pareto curve for these two objectives. In particular, an improvement of 70.58% in $F_{GRADUAL}$ implies a deterioration of 67.78% in the value of the function F_{EQUITY} . However, for medium values of the cost, no evident conflict exists, since a single solution (orange point) appears in the graph. In the case of high-cost values (red points), there is also a conflict, although to a lesser extent, in optimising ecological and social goals, leading to an improvement of 50.53% in $F_{GRADUAL}$, while deteriorating up to 104.30% the objective function F_{EQUITY} . The latter behaviour can be represented in a trade-off indicator defined as the ratio between the improvement of $F_{GRADUAL}$ and the deterioration of F_{EQUITY} , leading to a trade-off of 1.04 and 0.48 for low and high costs, respectively. For example, a value of 1.04 implies that $F_{GRADUAL}$ improves 1.04% by deterioration of 1% of F_{EQUITY} .

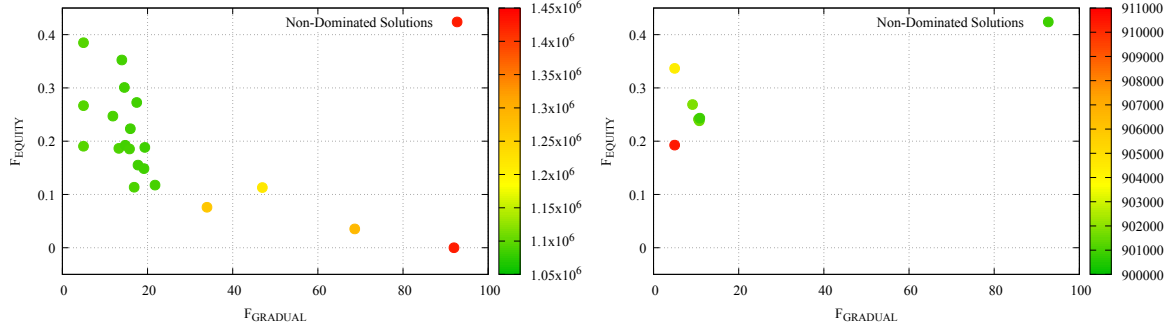


Figure 18: Projection in $F_{GRADUAL} \times F_{EQUITY}$ of the Pareto front approximations for instances A and B of the SBFR problem.

In the case of allowing the purchase of new and used buses, a lower number of non-dominated points was found in the Pareto front approximation. For this case (see the right panel of Figure 18), there is also a conflict between optimising the social and ecological goals at low costs, since we obtain a trade-off indicator of 0.257. On the other hand, for medium and high costs, there is no conflict between the optimisation of both objectives.

As shown by the results of our optimisation approach, it is possible to analyse the conflict between the optimisation of economic, ecological, and social metrics during the design of an electromobility adoption plan in public transportation networks. Moreover, bearing in mind that each point of the Pareto front approximations shown in this section is a long-term planning solution, the next section details what happens in that plan for solutions that benefit one objective over the others.

4.3.4 DETAILED NON-DOMINATED SOLUTIONS

In this section, we analyse the three solutions obtained while optimising each of the objective functions for instances A (purchase of only new vehicles) and B (purchase of new and used vehicles). We recall that a single solution represents a distinct planning scheme over the years, characterised by unique features and trade-off. By examining these solutions, we aim to provide decision makers with actionable insights to support informed choices aligned with their strategic priorities.

Figure 19, exhibits the total costs for the three solutions of instance A (dashed lines) and B (solid lines). It can be noted that, for instance **B** (see solid lines), annual costs consistently fall within the [18.6, 58.7] million dollar range, regardless of which objective achieves the minimum value. In contrast, for instance **A** (see dashed lines), the range of the total cost is [18.5, 369.8], indicating a notable variation in costs because during certain

periods, a significant number of vehicles are acquired, primarily due to the lifespan of the buses. Furthermore, we observe that in the case where the best value for F_{EQUITY} is achieved by purchasing only new vehicles (see dashed blue line), a substantial initial investment is required. In contrast, for the other scenarios, the initial investment is not as high (see dashed green and red lines), indicating that the acquisition strategy significantly influences the total costs. We highlight that costs are reduced when opting for the purchase of used vehicles. However, despite the potential financial benefits, operators rarely adopt this approach due to factors such as vehicle life expectancy, maintenance requirements, and operational uncertainties. These considerations often lead decision makers to prioritise the acquisition of new vehicles, despite the higher initial investment.

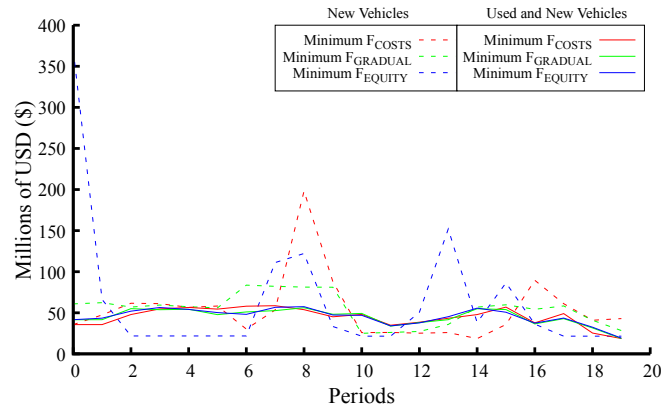


Figure 19: Total costs over time for selected solutions of instances A) Purchasing only New Vehicles and instance B) Purchasing both Used and New Vehicles.

Furthermore, when analysing the percentage of electrified lines in each period, we can see in Figure 20 that the transport network reaches electrification 100% between years 8 and 10, regardless of the priority objective (costs, equity, environmental) or the acquisition strategy (purchasing only new vehicles or purchasing both new and used vehicles). This indicates that the electrification goals of 100% can be achieved in half (or less) of the time set to plan the purchase.

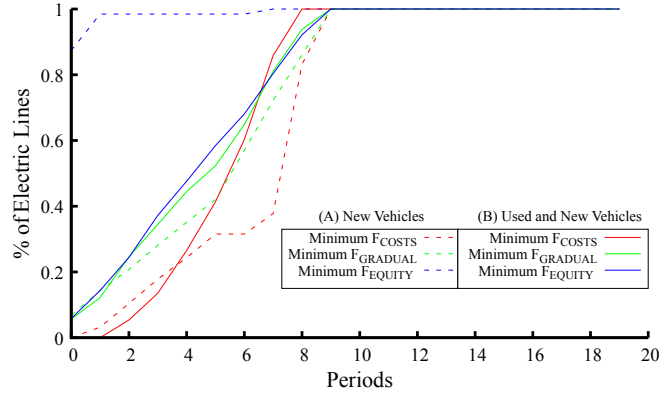


Figure 20: Percentage of lines electrified per period for each selected solution in instance A) Purchasing only New Vehicles and instance B) Purchasing both Used and New Vehicles.

To assess equity in the allocation of electric vehicles across the different regions of the city’s public transport network, we employ the Gini index (Gini, 1912; Ceriani and Verme, 2012). The Gini index is a standard measure of inequality, ranging from 0 (perfect equality, where all regions receive an equal share of electric vehicle coverage) to 1 (maximal inequality, where a single region receives all coverage). In this study, it is calculated based on the percentage of kilometres covered by electric vehicles within each region for each planning period. As such, the Gini index provides a quantitative measure of disparities in the distribution of electric vehicles, allowing the identification of regions that are over- or under-served by electromobility.

Figure 21 illustrates the behaviour of the Gini index during planning periods. The scenarios in which an equal distribution of electromobility between different regions occurs more rapidly are those in which F_{EQUITY} is optimised (see the dashed and solid blue lines), which aligns with the intended representation of our model. However, there is a significant difference between instances A and B, since it is possible to obtain a quasi-egalitarian distribution of electric vehicles in the city in period 2, when assuming purchasing only new vehicles. An interesting observation arises when considering the minimum value of F_{COSTS} for instance **B** (see solid red line). In this case, by period 9, the distribution is already fully equitable. However, in the periods preceding period 7, inequality reaches its highest levels in all scenarios. This suggests the need to evaluate whether prioritising a fully equitable distribution at a faster pace is preferable, even if it involves significant disparities in the earlier stages.

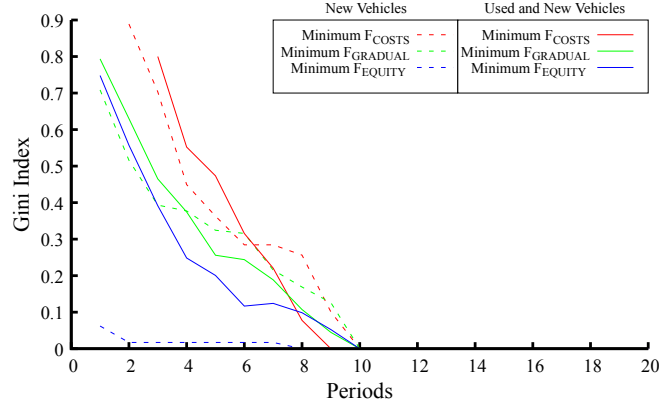


Figure 21: Gini index of each planning period for selected solutions of instance A) Purchasing only New Vehicles and instance B) Purchasing both Used and New Vehicles.

In summary, the experimental results in this section illustrate how the trade-off between the three objectives impacts the electromobility adoption plans, providing valuable information for decision making. Finally, we highlight that, in addition to analysing the details of the generated plans, our tool also helps identify policy implications and insights based on different contextual factors, such as period management (e.g., significant investments at the end of government terms) or technological advancements (e.g., cost reductions), which will be further illustrated in the next section.

4.4 MANAGERIAL INSIGHTS INTO MANAGEMENT OF TRANSPORT SYSTEMS DURING THE TRANSITION TO FLEET ELECTRIFICATION

Effective policy management is essential in the transition to electric vehicles (EVs), and our optimisation method offers a valuable asset in shaping these policies. In particular, our method assists in evaluating risk through simulation of different scenarios, offering a comprehensive perspective on potential impacts during the electromobility transition plan. This involves analysing uncertain elements such as technological advancements and costs related to electric buses, batteries, and charging infrastructure.

4.4.1 ASSUMING COSTS REDUCTIONS

First, we simulate an annual 2.5% decrease in electromobility costs by assuming only the purchase of new vehicles (instance A). Our aim is to provide policymakers with insight on how these gradual cost declines affect key metrics over time. This method improves the

understanding of the long-term impact of policies and facilitates more informed decision making. In Figure 22 we show the non-dominated solutions generated for both instances highlighted with circles for the base instance and triangles for the reduced cost scenario. We emphasise that, in the reduced costs scenario, the trade-off indicator's values between $F_{GRADUAL}$ and F_{EQUITY} stand at 2.16 for the low costs case and 0.83 for the medium costs case. Additionally, only one non-dominated solution is observed for high-cost values (see the red triangle).

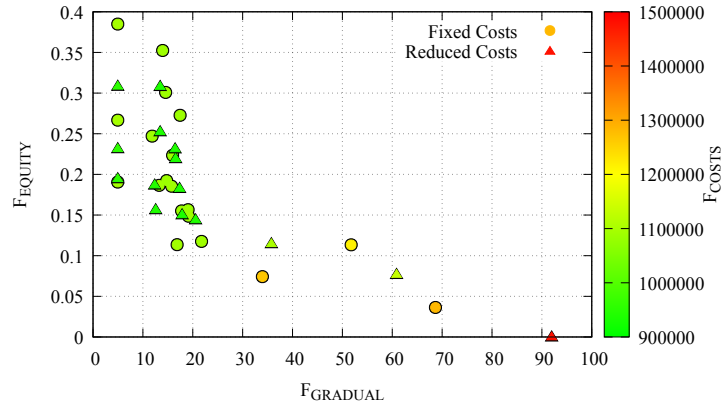


Figure 22: Pareto optimal solutions projected on the Cartesian plane $F_{GRADUAL} \times F_{EQUITY}$ for both the original instance A and for instance A with an assumed gradual decrease in costs.

We compare the base instance and the scenario with a gradual reduction in capital costs of adopting electromobility, and we can observe that when optimising F_{COSTS} the total costs assuming gradual reductions ranges within $[933277, 1478950]$ compared to the range $[1082350, 1283090]$ in the base scenario, leading to an improvement of 13.77% in the minimal cost. Moreover, the minimal value of $F_{GRADUAL}$ is the same in both scenarios, while we obtain an improvement of 19.87% in F_{EQUITY} when solving the scenario with reduced cost compared to the base instance.

We recall that besides analysing the trade-off between economic, ecological, and social objectives, our optimisation approach provides the details of adoption plans for electromobility in public transport systems. In response to the latter, Figure 23 shows the plan of solutions that optimise each objective function for both scenarios. First, the total costs assuming the gradual reduction of costs are lower compared to the original instance (see the red lines in case (a) of Figure 23. The gradual electrification of the systems has a similar behaviour in both cases (see green lines in case (b)). Finally, both cases present a rapidly egalitarian distribution of electric buses along the different regions while optimising F_{EQUITY} (blue lines in case (c)), in particular, since the beginning of the

planning period assuming a gradual reduction of costs (blue line is in the value of 0 of vertical axis) and in period 2 in the case of the original instance (see dashed blue line).

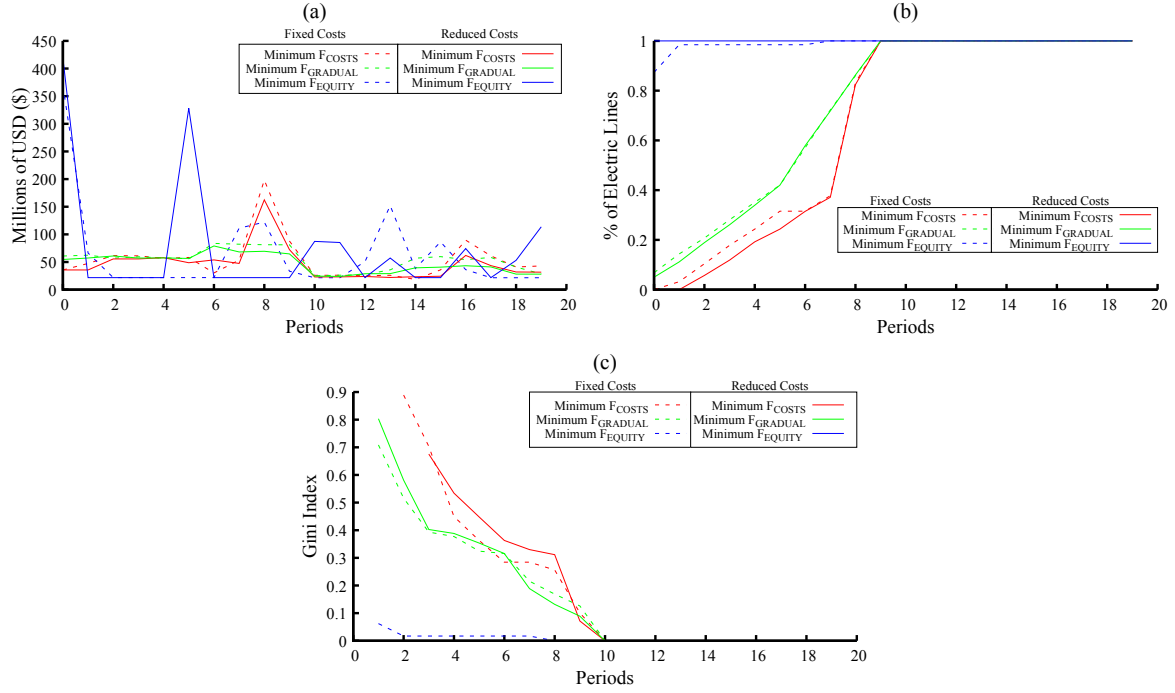


Figure 23: Plans for adopting electromobility concerning non-dominated points derived from optimising each objective function within SBFR.

Our study underscores the critical role of assessing evolving cost reductions when designing policies for the adoption of electromobility. The findings indicate that a steady decrease in costs can yield substantial economic benefits while simultaneously improving equity and improving system stability over the long term. Furthermore, our optimisation framework is versatile and can be adapted to investigate other policy strategies, such as assessing the outcomes of setting administrative deadlines alongside major investments in designated planning intervals, replicating situations where governments provide significant funding to accelerate fleet electrification. In addition, the model could incorporate policies on emissions penalties for private operators within the public transport sector to assess their economic and operational effects. These enhancements would allow policymakers to foresee possible obstacles, evaluate different regulatory approaches, and formulate more flexible transition strategies that are in line with long-term sustainability objectives.

4.5 CHAPTER SUMMARY AND REMARKS

The results presented in this chapter highlight the potential of multi-objective optimisation as a valuable decision-support tool for public transport authorities and policymakers. By simultaneously balancing economic feasibility, environmental performance, and social equity, the proposed framework contributes to the design of more sustainable and inclusive urban transportation systems. The analysis also underscores that, while fleet electrification offers clear environmental benefits, its economic and spatial implications necessitate careful, coordinated planning and prioritisation. Ultimately, the methodological approach developed in this study provides a comprehensive and adaptable foundation for future strategies aimed at achieving carbon-neutral and equitable urban mobility. The main conclusions and prospective research directions arising from this work are discussed in detail in Section 5.2 of this thesis.

CONCLUSIONS AND FURTHER RESEARCH AREAS

This chapter summarises the main findings and contributions of the research presented in this thesis, while outlining potential directions for further investigation. Two distinct projects were addressed: the first focused on the estimation of public transport origin-destination matrices (ODMs) using optimisation models with multiple data sources, and the second on the sustainable transition of bus fleets from diesel to electric vehicles through multi-objective planning. The chapter highlights the methodological advancements, practical implications, and insights gained from each study, and provides a synthesis of the lessons learned and opportunities for future research in urban public transportation planning.

5.1 ORIGIN-DESTINATION MATRIX ESTIMATION

In this study, we proposed four bi-level mathematical models to estimate an ODM of public transport. At the upper level, the models decide the passengers for each OD pair, while the lower level determines the transit assignment problem, minimising total travel times. Our proposed models consider a combination of different types of information as an outdated ODM, observed flows, boarding/alighting data, and structure of the outdated ODM and passenger flows to guide the optimisation phase through different objective functions in the upper level and different constraints.

We performed a comparative analysis based on different amounts of information for each information type, and the optimisation model and numerical results show that using complete information does not necessarily lead to the best results. Moreover, comparing our models based on different information types leads to the following conclusions.

- Considering structural properties of the demand and flows and hard constraints for boarding and alighting leads to finding the best estimations of the ODM (Model D).
- Considering only soft constraints of structural properties (Model B) results in solutions even worse than not considering any of them (Model A).
- Considering a model with only hard constraints of boarding and alighting (Model C) is better than the previous two models (Model A and B).

Regarding future research directions, we should explore methods to enhance the accuracy of our estimations by incorporating additional data sources. For instance, we could integrate partial OD flows (as in Behara et al., 2022; Pamula and Zochowska, 2023; Parry and Hazelton, 2012; Patil et al., 2023; Rostami Nasab and Shafahi, 2020), or route frequency usage for passengers with AFC (or more detailed demand information over time). Another further research area is determining which segments of lines and stops are most relevant to observe, thus enhancing our model estimations (such as Yang and Zhou, 1998). Furthermore, exploring the utilisation of more complex assignment models could be beneficial. This exploration would involve assessing whether the results obtained in our study remain consistent when considering different assignment models, thus refining our understanding of the impact of incorporating certain types of information in both the objective function and constraints. Moreover, comparisons of estimated and exact demand values for OD pairs in Appendix A show that model D is efficient in estimating the demand on the tested instances. Finally, we could focus on extending the optimisation problem to estimate OD matrices assuming network reconfigurations (which are necessary as shown in Appendix B), including different sets of routes, stops, or infrastructure. This is relevant due to various mobility policies that adapt to urban development in cities with growing populations.

5.2 SUSTAINABLE ELECTRIC BUS FLEET REPLACEMENT

This research introduces a multi-objective optimisation model for the sustainable transition of bus fleets from diesel to electric vehicles within public transportation networks. The framework incorporates economic, environmental, and social objectives to aid in the decision-making about fleet electrification. By reducing operational expenses, improving fleet electrification, and ensuring a fair distribution of electric buses in urban areas, the model serves as a valuable resource for public transportation operators and policymakers. The findings reveal the economic practicality of switching to electric buses by highlighting

long-term savings in fuel, maintenance, and battery replacement. The use of pre-owned electric vehicles helps lower initial expenditures, supporting adoption by operators with limited budgets. Ecologically, gradual electrification of the fleet leads to substantial reductions in greenhouse gas emissions and improves urban air quality. The phased approach balances environmental advantages with operational practicability. Furthermore, ensuring an equitable allocation of electric buses ensures that all communities experience the benefits of reduced noise and improved air quality, which is essential for cities with varied socioeconomic demographics.

The use of the ε -constraint algorithm allows decision makers to analyse trade-off between cost, electrification, and equity. Pareto front approximations provide a clear visualisation of these relationships, enabling informed decisions based on strategic priorities. Furthermore, the study highlights the importance of considering technological advancements and the progressive reduction of costs in policy design. Simulation of scenarios with gradual cost reductions in electrification shows that such strategies can lead to significant improvements in both economic and environmental metrics.

For future research, it would be relevant to explore the integration of renewable energy sources, such as solar or wind, into the charging infrastructure, which would further enhance the sustainability of electric fleets. Incorporating real-time optimisation techniques would allow dynamic adjustments to fleet operations based on demand, energy availability, and traffic conditions, improving operational efficiency. Furthermore, extending the model through robust and stochastic optimisation approaches would address uncertainties related to energy price fluctuations, advances in battery technology, and changes in regulations, enhancing the adaptability of the solutions. The model could also be expanded to assess the impact of additional policy measures, such as emissions penalties for private operators or incentives for early adoption of electric buses, providing a more comprehensive view of the economic and operational implications of different regulatory scenarios. Finally, applying the model to cities with varying population densities, geographic configurations, and socioeconomic conditions would allow evaluation of its scalability and adaptability, generating valuable insights for its implementation in diverse urban contexts.

APPENDIX A

ANALYSING ODM AND PASSENGERS FLOW ESTIMATION IN MODEL D

In this section, we present a comparison between the estimated demand and the exact demand, as well as the estimated flow and the observed flow, for model D, which experimentally demonstrated to obtain, on average, better estimations for all classes of instances tested using an information level of $|\bar{A}| = |A^L|$ and $|\bar{N}| = |N^L|$ (that is, making observations at all the line segments and all the stops). In particular, our comparison is conducted using a scatter plot, one for the demand and another for the segment flows. For the demand, we plot the points $(\bar{g}_k, \mathbf{g}_k)$ for all $k \in K$, while for the segment flows we plot $(\bar{v}_a, \sum_{k \in K} (\mathbf{v}_a^k + \mathbf{v}_{t(a)}^k))$ for all $a \in A^L$. Ideally, our estimations should be equal to the exact or observed information, meaning the closer the points are to the identity line (the straight line passing through the origin (0,0) with a slope of 1), the better.

We take one instance for each type of variation, i.e., increasing demand (Figure 24), decreasing demand (Figure 25), and both (Figure 26). To analyze the most unfavourable case for our estimation approach, we consider the case where all entries of the OD matrix change.

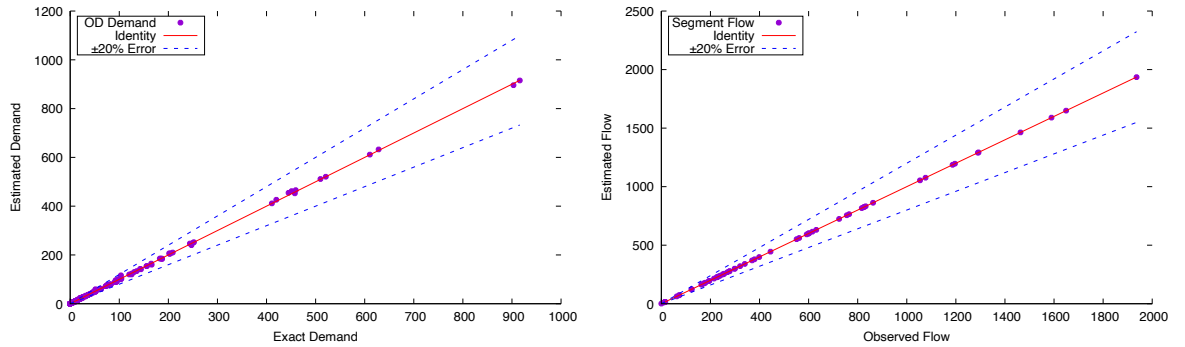


Figure 24: Comparison of estimated and exact passenger demand and passenger flow for instance *Incr_100%*.

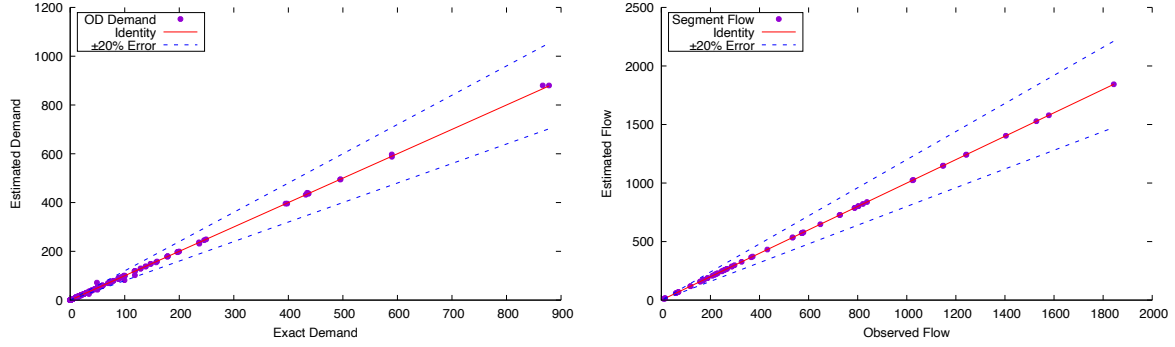


Figure 25: Comparison of estimated and exact passenger demand and passenger flow for instance *Decr_100%*

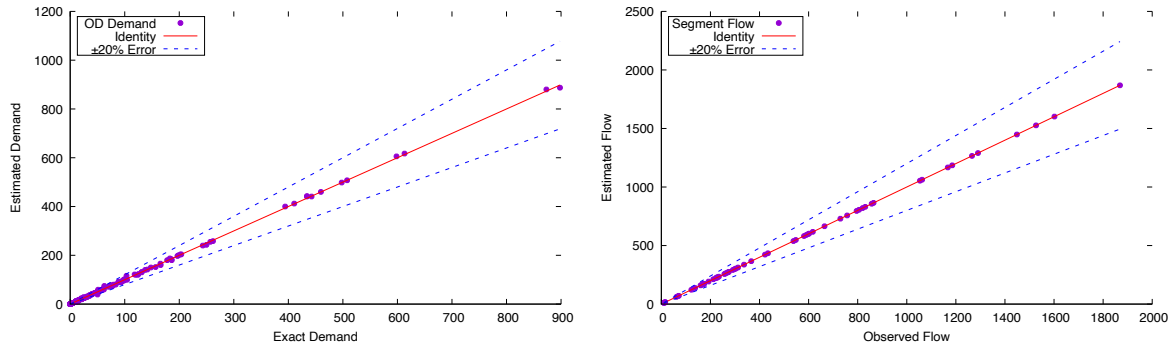


Figure 26: Comparison of estimated and exact passenger demand and passenger flow for instance *Both_100%*

Notice that Figures 24–26 exhibit a great similarity (fit to the line with a slope of 1) for the estimated and exact/observed values of demand and passenger flows.

In addition to performing the comparison for the case of observing 100% of the line segments, we also show the results with an observation level of 50% (and 100% of the stops). The results are presented below, where we can see that although there are significant differences between estimated and observed flow only on a few arcs, the similarity between estimated and exact demand prevails.

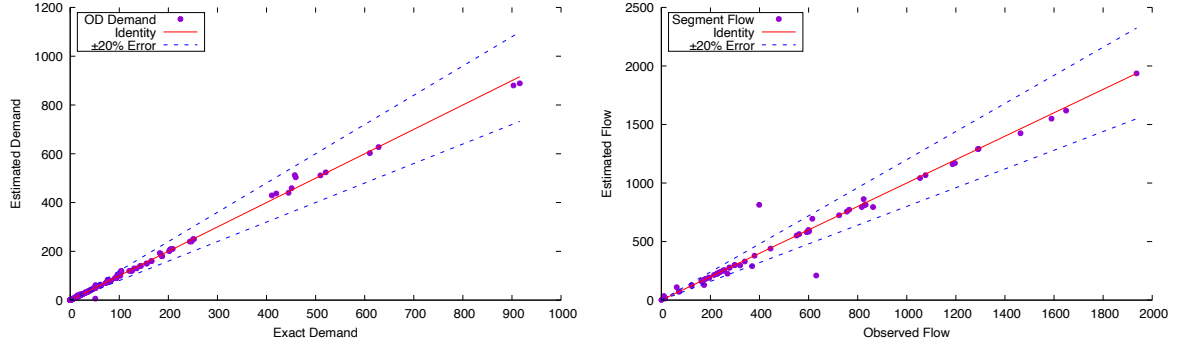


Figure 27: Comparison of estimated and exact passenger demand and passenger flow for instance *Incr_100%*, but using only 50% of observed flows.

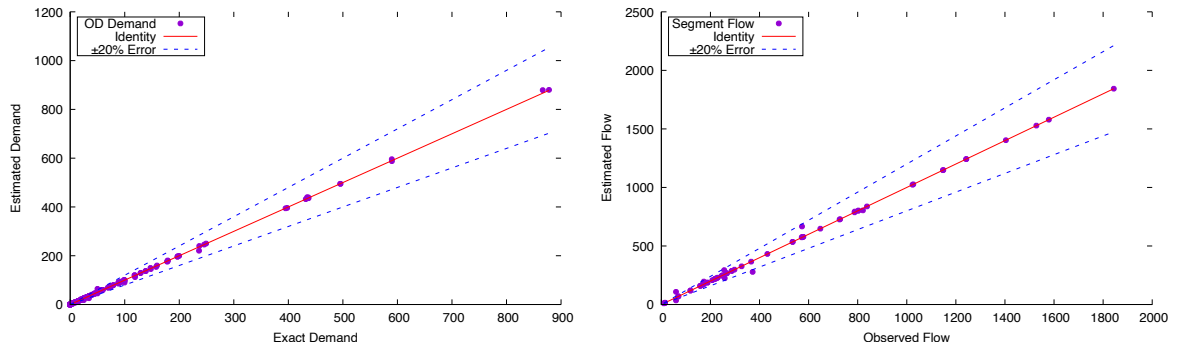


Figure 28: Comparison of estimated and exact passenger demand and passenger flow for instance *Decr_100%*, but using only 50% of observed flows.

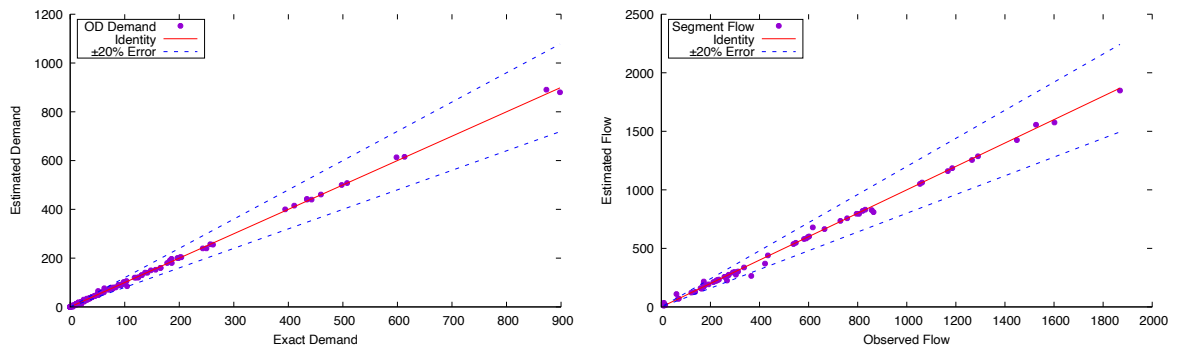


Figure 29: Comparison of estimated and exact passenger demand and passenger flow for instance *Both_100%*, but using only 50% of observed flows.

The above results reinforce our conclusions about the usefulness of optimisation models and different types of information for estimating Origin-Destination matrices.

APPENDIX B

ANALYSING OUR MODEL ASSUMING CHANGES IN THE TRANSIT NETWORK

In addition to changes in passenger demand for different origin-destination pairs, other changes that may occur over time include the reconfiguration of the transport network in terms of stops of transit lines. This is especially true in scenarios of cities with a high level of change due to land use trends, socio-economic activities, and even those recurrently affected by disasters. In this context, we conducted an experiment to evaluate our model by assuming that at the time of taking the outdated demand information, one line was missing, as shown in Figure 30.

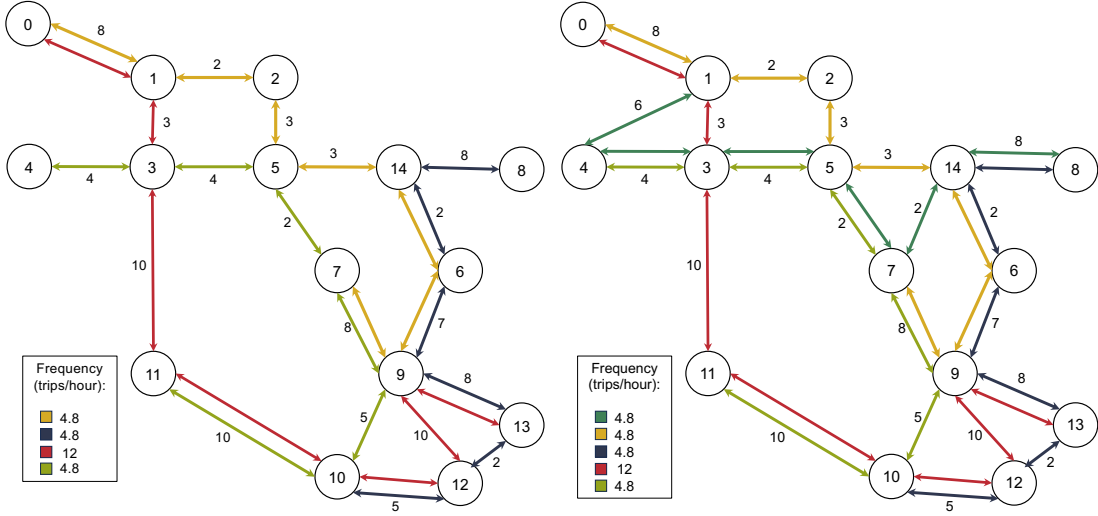


Figure 30: Old and new sets of transit lines to analyse our model D, assuming changes in the transport network.

Based on the latter scenario, model D was implemented on the instances described in Appendix A assuming a 100% level of observed flows. The results are shown in Figures 31–33.

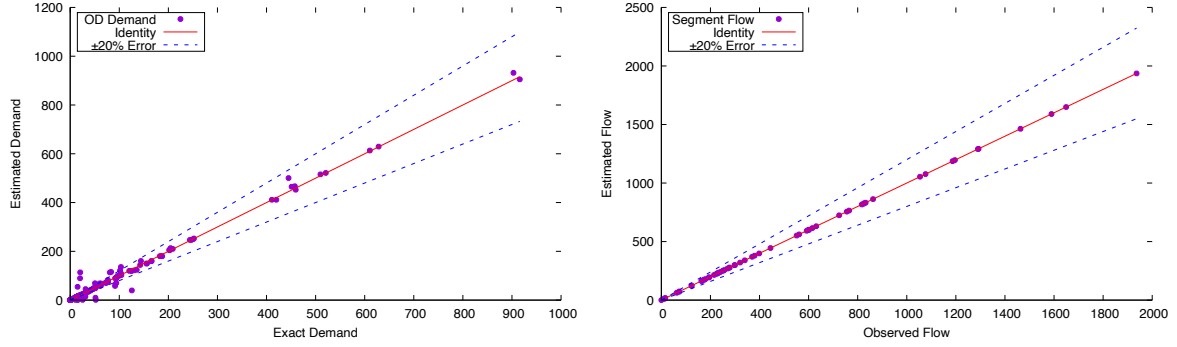


Figure 31: Comparison of estimated and exact passenger demand and passenger flow for instance *Incr_100%*, using 100% of observed flows.

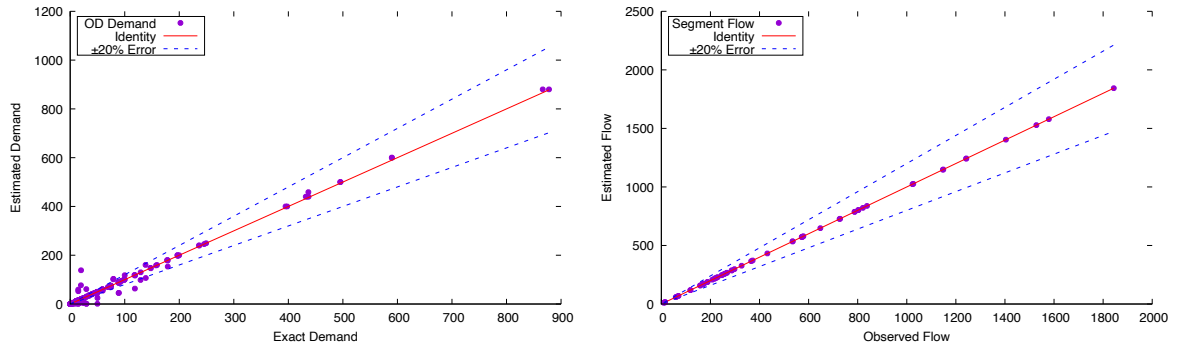


Figure 32: Comparison of estimated and exact passenger demand and passenger flow for instance *Decr_100%*, using 100% of observed flows.

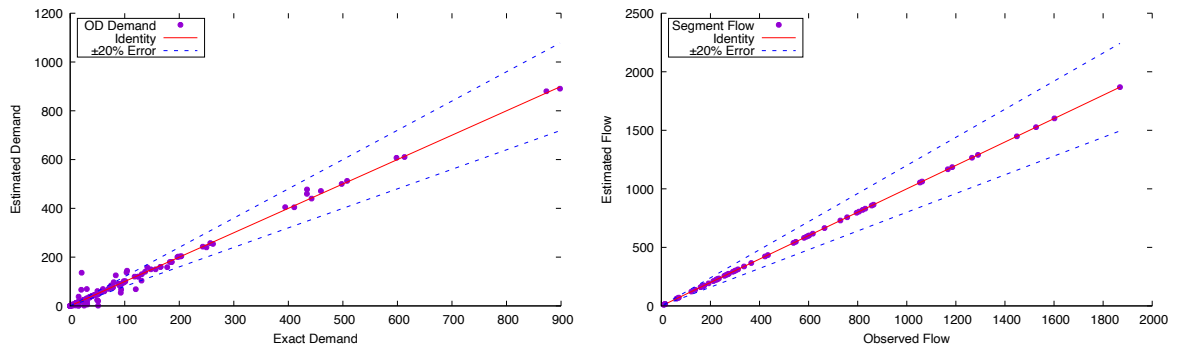


Figure 33: Comparison of estimated and exact passenger demand and passenger flow for instance *Both_100%*, using 100% of observed flows.

Note that the flow estimation resulting from our model is of good quality. However, there is a deviation of more than 20% between estimated demand and actual demand for a few OD pairs (less than 13.33%). These aforementioned results indicate that the model needs to be enhanced to address changes in the transport network.

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