Finding Solutions for Complex Systems:
Saving Traction Energy in Rail

BY

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A thesis submitted to the

University of Birmingham for the degree of

DOCTOR OF PHILOSOPHY

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March 2017

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Abstract

The author of this thesis presents a novel method for evaluating solutions for complex systems, which is demonstrated with an application to the problem of traction energy saving in rail.

Complex optimisation problems, which are concerned with maximising or minimising a given aspect of a complex system, such as time, energy or cost, are very difficult to solve. Often a range of solutions already exist and the difficulty lies in determining which of the available solutions to implement in which part of the system. As part of this study, a method has been developed that allows the solver to overcome the key challenges in: defining the parts of the system (subsystems); minimising the model complexity; quantifying the effectiveness of solutions; and identifying the relationships between solutions and subsystems.

Firstly complex systems are defined and the current approaches to complex problem solving are introduced. Following on from this, relevant sensitivity analysis, data visualisation and data analysis techniques are presented. The developed method is then discussed in detail, including the limitations of its application. The given system is broken down into a number of subsystems, and then a sensitivity analysis is performed on a numerical model of each subsystem to determine the best solutions for each of them individually. This approach not only allows the most suitable solutions for each subsystem to be identified, but also allows the relationships between subsystems to be analysed, thereby providing insights into the whole system behaviour. The individual subsystem results can then be used to inform in-depth simulations of appropriate solutions.

The effectiveness of the method is demonstrated through its application to the problem of traction energy saving in rail. Subsystems are defined based on the network and service characteristics of the railway. Six solutions to reduce traction energy are investigated, as well as the effect of gradient and interstation distance on solution suitability. For each subsystem, Principal Components Analysis is used to evaluate the trends between solutions and Trend Identification Plots are introduced as a way of visualising the relationship between each solution and the energy and journey time Key Performance Indicators. Following the

individual subsystem analyses, the relationships between subsystems are explored using a variety of visualisation techniques.

The analysis determines that the suitable solutions differ between different types of railway, thus providing information for operators about which solutions should be targeted. The system analysis provides further information about the relationships between subsystems and how the effectiveness of solutions changes with service and network characteristics. Based on the system results, an in-depth simulation of the implementation of Permanent Magnet Synchronous Motor technology is conducted, illustrating the suitability of the method as a tool to inform further studies.

Acknowledgements

"A great discovery solves a great problem, but there is a grain of discovery in the solution of any problem. Your problem may be modest, but if it challenges your curiosity and brings into play your inventive faculties, and if you solve it by your own means, you may experience the tension and enjoy the triumph of discovery."

G. Polya (1973)

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List of Acronyms

Acronym	Short for
ATO	Automatic Train Operation
BE	Braking Effort
DAS	Driver Advisory Systems
DOE	Design of Experiments
EE	Elementary Effects
EMU	Electric Multiple Unit
ESS	Energy Storage System
FAST	Fourier Amplitude Sensitivity Test
FCFDS	Feasible Conceptual Future Desirable Situation
HS	High Speed
HS1	High Speed One
HVAC	Heating, Ventilation, Air Conditioning
IGBT	Insulated Gate Bipolar Transistor
IM	Induction Motor / Machine
KPI	Key Performance Indicators
MA	Multivariate Analysis
OFAT	One Factor at a Time
OLE	Overhead Line Electrification
PC	Principal Component
PCA	Principal Components Analysis
PMSM	Permanent Magnet Synchronous Motor
ROSCO	Rolling Stock Operating Company
SA	Sensitivity Analysis
SiC	Silicon Carbide
SOI	System of Interest
STS	Single Train Simulator
TE	Tractive Effort
TIP	Trend Identification Plot
TOC	Train Operating Company
TSI	Total Sensitivity Index
TSS	Total Sum of Squares
VVVF	Variable Voltage, Variable Frequency
WESS	Wayside Energy Storage System
UU	Urban Urban
UComm	Urban Commuter
ICComm	Inter-city Commuter
ICHS	Inter-city High Speed
HSComm	High Speed Commuter
HSHS	High Speed High Speed

Chapter One

Introduction

"Begin at the beginning," the King said, very gravely, "and go on till you come to the end: then stop"

<div align="right">L. Carroll (1865)</div>

How can we get to work faster? Or save the planet from global warming? Or cure cancer? Although these problems appear unique, they are all fundamentally optimisation problems concerning complex systems: in these cases, our transport modes, our planet and our bodies. A complex system can generally be defined as containing many interconnected parts, which exhibit self-organisation and emergent behaviour (Ladyman et al., 2013). Commonly, for optimisation problems of this type, solutions already exist and the real problem is determining which of these existing solutions are best to reach our goal, or indeed, goals. For example, should we travel by bus, car, cycling, running, walking, flying or should we use a combination of these modes? Flying reaches the greatest speeds, but it would not necessarily be practical for a 10 kilometre journey. Evaluating solutions within the context of the system, therefore, is extremely important. But we often cannot do this in the real world, due to expense or time constraints, not to mention external factors which may influence the experiments (in this case traffic, weather or physical fitness). What is needed is a computational model, which allows us to test all possibilities and to compare them. However, if everything is interconnected, what do we include or remove? Is it feasible to create one big model with the computational power and resources currently available to us? Even if the model were created, what if the experimental outcomes are either too complex or too simple to allow us to comprehend the trends and relationships between the system parts?

In the study that follows I propose a screening method to be used in the first instance to find the most appropriate solutions for complex systems. The given system is first broken down into a number of subsystems and then a Sensitivity Analysis is performed on a numerical model of the subsystems to identify the best solutions for each of them individually. The complexity of the original model is reduced by omitting irrelevant factors, thereby reducing the computation time and improving the clarity of the results. This approach allows for the

analysis of the interactions between the subsystems of a system, giving insights into the behaviour of the system as a whole. The individual subsystem results can be used to inform in-depth modelling of appropriate solutions, and the application of traditional techniques to optimise each solution in turn.

Although I have not found the best approach to get to work, save the planet from global warming or cure cancer in this thesis, I believe this study to be a worthwhile step forward in the approach used to solve complex problems. The proposed method is applied, as proof of concept, to the somewhat simpler example of saving traction energy in rail.

1.1 Purpose of the Research

The purpose of this research is to develop a screening method to evaluate solutions for complex systems and to demonstrate the suitability of the method through an application to the issue of traction energy saving in rail. Specifically, this method is applicable to complex problems which are concerned with optimising a given variable – time, energy, cost, ability – using solutions that are already in existence. The system must be capable of being broken down into comparable subsystems, and of being modelled numerically. The inputs and outputs of the system must also be quantifiable, not qualitative, in order to allow statistical methods to be used for the analysis.

Rail is a good example of such a system. Featuring a range of different network and service types, it lends itself to being broken down into subsystems, each of which can be modelled numerically in terms of their characteristics. The fundamental equation of motion, which governs all transport modes, is the core of the numerical system model. The question of energy saving in rail is topical as the sector is experiencing rapid growth across the world, whilst also being required to reduce energy consumption and carbon emissions (European Commission, 2011). Within the UK, projects such as High Speed 2 (HS2 Ltd., 2015), High Speed 3 (National Infrastructure Commission, 2016), Crossrail (Crossrail, 2017) and Network Rail's Electrification Programme (Network Rail, 2017) are testament to the importance of rail in order to meet transport demand in an environmentally concerned economy.

A secondary purpose of this research is to investigate which multi-variate analysis methods and data visualisation techniques are most appropriate for comparing the results of multiple subsystems and identifying the relationships within and between them. Visual data representations take advantage of the ability of humans to perceive patterns and thereby draw insights and conclusions from the data, far better than from studying numerical results. Such visualisations also connect the user to the experimental process, allowing them to redefine the experimental parameters and goals as appropriate (Keim, 2002).

1.2 Research Objectives

The main aims of this research project are as previously stated:

- To develop a screening method to evaluate solutions for complex systems

- To demonstrate the suitability of the method with an application to the example of traction energy saving in rail

In order to meet these aims, complex systems and the approaches to solving problems concerning them must be understood first of all. Additionally, thought must be given to how data is represented before the method design stage, to ensure the data captured is appropriate and allows both the results and trends between subsystems to be identified easily. The four research objectives are given in Table 1, alongside related research questions and the chapters which cover these objectives.

Table 1: The research objectives and related research questions of this thesis

Objective		Research Questions		Chapters
1	To understand complex systems and the approaches to solving complex problems	a.	What are complex systems and problems?	2
		b.	How are solutions for complex problems found?	
2	To determine appropriate experimentation and data visualisation methods for complex systems	c.	How is multidimensional data visualised and analysed?	3
3	To develop a method to find solutions for complex systems	d.	How are subsystems of systems defined?	4
		e.	How is solution suitability determined?	
		f.	Which data should be captured by the method?	

		g.	How is data kept consistent between subsystems?	
4	To demonstrate the suitability of the screening method and data visualisation techniques, through application to the example of traction energy saving in rail	h.	How can the method be applied in practice?	5-6
		i	How can the results be used?	7
		j.	How might the method be used in the future?	8

1.3 Hypotheses

Formalising the approach to complex optimisation problems will allow meaningful conclusions to be made about: where particular solutions are most appropriate to be implemented within the system; how the subsystems relate to one another when the whole system is considered; and what further experimentation that should be completed, i.e., in-depth simulations of solutions.

The three key questions within this hypothesis are tested specifically by the three sub hypotheses below, which relate to the test case of energy saving in rail:

- Do the solutions appropriate for particular railways differ depending on the network and service characteristics of the given railway?

- Can these differences be used to determine the relationships between the different networks and services?

- Can the results be used to inform further experiments?

1.4 Thesis Structure

This section briefly describes where the objectives, research questions and hypotheses are explored within the thesis chapters.

Chapters 2 and 3 are literature review chapters, which address research objectives 1 and 2 respectively. Chapter 2 provides background information defining complex systems and introduces approaches to solving complex problems, addressing research questions a. and b. Chapter 3 covers Sensitivity Analysis (SA) methods which can be used to evaluate complex system behaviour, and different techniques for visualising and analysing the multi-variate data generated by these analyses, that is, research question c.

Chapter 4 describes the 8-stage method which has been developed in this study, including its objectives and scope. Research questions d-g are answered in detail.

In Chapters 5 and 6 the method is applied to the problem of reducing traction energy in railways. Chapter 5 covers stages 1-4, which can be thought of as the background of the problem, including a review of the solutions currently available; the definition of distinct railway subsystems; and a description of the simulation model. Chapter 6 then describes the implementation of the SA, and the subsystem and system analyses. The three sub-hypotheses are also explored within Chapter 6. These chapters together address research question h.

Chapter 8 addresses research question i. by providing an example of how the SA findings can be used to inform new experiments and in-depth simulations. A feasibility study on the implementation of Permanent Magnet Synchronous Motor (PMSM) technology is performed.

Chapter 9 concludes the thesis by discussing the implications of the research, the key achievements and considerations for further work, including how the method might be altered to address different problems, that is, research question j.

1.5 Publications

Prior to completing this thesis, I published three peer-reviewed journal papers and two conference papers as lead author and contributed to another conference paper as a secondary author. This section gives details of how these papers are used within the thesis. The first pages of all of the papers are included in Appendix A. Please note that Douglas is my maiden name, and that these papers were published prior to my marriage in January 2017.

1.5.1 Contributing Publications

Portions of my previous publications are reproduced within the body of this thesis in Chapters 3, 5 and 7, in line with the journal publishing agreements. Copies of the agreements are included in Appendix B. Passages which are an exact match are indicated in italicised black or grey text, and a key is provided at the beginning of each of the respective chapters.

1. Douglas, H., Roberts, C., Hillmansen, S. and Schmid, F., 2015, *An assessment of available measures to reduce traction energy use in railway networks*, Energy Conversion and Management, 106(2015), pp.1149-1165

2. Douglas, H., Roberts, C. and Hillmansen, S., 2016, *Method to evaluate solutions for complex systems: rail energy*, Proceedings of the Institute of Civil Engineers – Transport, 169(5), pp. 283-297

3. Douglas, H., Schmid, F., Roberts, C. and Hillmansen S., 2016. *Evaluation of Permanent Magnet Motor Energy Saving Technology for Different Types of Railways*, IEEE International Conference on Intelligent Rail Transportation, Birmingham, UK, 23-25 August 2016, pp. 123-129

1.5.2 Relevant Publications

These publications are relevant to the project, and appropriately referenced within the work:

4. Douglas, H., Weston, P., Kirkwood, D., Hillmansen, S. and Roberts, C., 2017, *Method for validating the train motion equations used for passenger rail vehicle simulation*, Proc IMechE Part F: J Rail and Rapid Transit, 231(4), pp.455-469

5. Douglas, H., Roberts, C. and Hillmansen, S., 2016, Optimising energy saving in metro systems through characteristic evaluation, IET International Conference on Railway Engineering, Brussels, Belgium, 12-13 May 2016, pp.1-12

1.5.3 Other Publications

I have contributed to another publication during the time of the research project, but this is not used or cited within this work.

6. Hamid, H., Nicholson, G., Douglas, H., Zhao, N. and Roberts, C., 2016/17, *Investigation into Train Positioning Systems for Saving Energy with Optimised Train Trajectories*, IEEE International Conference on Intelligent Rail Transportation, Birmingham, UK, 23-25 August 2016, pp. 460-468

Chapter Two

Literature Review

"There is always a well-known solution to every human problem – neat, plausible and wrong."

H.L. Mencken (1920)

2.1. Introduction

In this chapter I address the first two research questions, namely, what are complex systems and how are solutions for complex problems found? Firstly, definitions of complex systems are discussed and the qualitative characteristics of emergence and complexity are presented as a way of defining complex systems. Complex problem solving is then introduced in the context of complex systems, and the two stages of complex problem solving, knowledge acquisition and knowledge application, are explored in detail.

2.2. Complex Systems

In order to write this sentence I am using a multitude of complex systems, from each of the cells in my body, to my brain, to the university computer network and the internet. Understanding these and other complex systems has become an integral part of research in disciplines ranging from physics, computer science and engineering, to sociology, psychology and economics. Although each of these subjects have their own examples of complex systems to explore, a range of interdisciplinary fields have also been created by the study of complex systems (Bar-Yam, 1997). But what precisely is a complex system?

The problem is that there is no single precise and concise definition. The Oxford English Dictionary[1] defines *complex* and *system* respectively as: consisting of many different and connected parts; and a set of things working together as part of a mechanism or an interconnecting network; a complex whole. However, these definitions are not especially useful, not least because the word complex is used to define a system.

A more complete description is given by Jacobson (2000, p.14):

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[1] All future definitions are taken from The Oxford English Dictionary, unless otherwise stated, and are shown in inverted commas, rather than quotation marks

"Briefly, complex systems may be characterized by the interactions of numerous individual elements or agents (often relatively simple), which self-organize at a higher hierarchical level of the system that in turn show emergent and complex properties not exhibited by the individual elements."

Within this definition two important concepts are introduced, which are absent from the standard definitions given before. These are: the interactions of the parts and their subsequent emergent behaviour, and the way in which the parts of a system self-organise within hierarchical levels. These attributes are often referenced in the literature as emergence and complexity respectively (Bar-Yam, 1997; Norman and Kuras, 2006), and can be considered as the two main characteristics of complex systems.

Revisiting the dictionary definitions, it is possible to have a system which is complex but for this not to be a complex system. I would argue that these should be referred to as complicated systems, rather than complex systems. The example used by Ottino (2004) is an elaborate mechanical watch. A watch consists of a number of connected parts and it is a system since these parts work together as part of a mechanism to tell the time. However, the behaviour of the system is predictable from the behaviour of its parts, and if one key part fails then the whole system fails. It therefore displays neither emergent behaviour, nor self-organisation, and as such cannot be a *complex system*. This example illustrates that just as the term *complex system* is more than the sum of its definitions, complex systems themselves are more than the sum of their parts.

2.2.1 Emergence

Emergence is defined as the 'process of becoming visible after being concealed; or of coming into existence or prominence'. In terms of complex systems then, emergence refers to the behaviours that exist for the whole system, but are not immediately visible when considering the behaviours of the system parts. This definition of emergence is often adopted in the domain of system-of-systems engineering (Stary and Wachholder, 2016; Fisher, 2006). I hope to highlight with this definition that the overall behaviours rely on the behaviours of the parts, but that the co-acting relationships between them are not obvious. Bar-Yam (1997, p.10.) states that "the collective behaviour is, however, contained in the behaviour of the parts, if they are studied in the context in which they are found".

The study of behaviour in context is crucial to developing understanding of complex systems, and is part of what makes problem solving for complex systems challenging. It is not enough to break the system down and study the parts individually, the whole system, or ensembles of parts, must be considered (Bar-Yam, 1997). This dramatically increases the scope of the investigation, and requires larger, multifaceted models which scale with the system complexity (however it is defined).

2.2.2 Complexity

Describing and quantifying complexity is… complicated[2]. Reconsider the elaborate mechanical watch. I have already stated that it is not a complex system because it lacks emergence, but does it exhibit complexity? That really depends on how complexity is determined: is it by the number of parts, the number of interactions between the parts, the simplicity of these interactions (and how simplicity is determined), the organisation of the system, or combinations of these and other measures?

2.2.2.1 The properties of complexity

The properties of complexity are extensively discussed by Ladyman et al. (2013) and the following are deemed to be necessary and sufficient for complexity to be present:

1. **Ensembles of many elements**

   Not only do there have to be many elements (parts), but these elements should be similar at each level of the hierarchical structure so information can be exchanged. For example, there are many similar planes at an airport and many similar airports across the country. "Ensembles of similar elements at one level form a higher-level structure which then interacts with other similar high-level structures" (p.28).

2. **Interactions**

   It is important not just that the elements interact, but that their states or behaviours depend on these interactions. For example, a plane may have to circle an airport before landing because there is no runaway available, due to other planes arriving.

3. **Disorder**

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[2] Complicated in this case is taken to mean 'involving many different and confusing aspects'.

Even though the interactions between elements are disordered, order is re-established by these interactions. The equilibrium state of a complex system therefore is dynamic, rather than static. Consider the railway as an example. If a delay occurs to a single train and you observe the system at an elemental level the reaction of each train will appear disordered. However, these disordered interactions can still lead to the recovery of the timetable.

4. **Robust Order and Memory**

Robust order refers to the formation of patterns from the disordered interactions discussed above. Extending the railway example, when a range of delays are considered, patterns can be found between the type of delay and the length of recovery time, even though the actions of the individual trains are disordered and may differ in every case. It is in this way that a complex system can be seen to exhibit memory.

The final two properties can be thought of as an extension of self-organisation, which Jacobson (2000) required to be present in complex systems. As previously stated, the watch does not self-organise and therefore cannot exhibit complexity.

2.2.2.2 Quantifying Complexity

Bar-Yam states that the level of complexity of a system can be loosely defined by "the amount of information required to describe it" (1997, p.12). This information is not only the description of each part of the system and how these parts interact, but also the description of the subsequent behaviours which emerge at system level. In this way, it is possible to describe complex systems both microscopically and macroscopically, where these descriptions refer to the state of the system elements and whole system state respectively. The microscopic state of the system is decided by the interactions of the ensembles of many elements, i.e. properties one and two, whereas the macroscopic state arises from the properties of disorder and robust order and memory.

In order to describe the complexity of the system at the correct level the macroscopic states must be considered first, and then the microscopic states which contribute to this state determined (Bar-Yam, 1997). In this way, the amount of information included in the description is minimised, as only the information necessary to describe the macroscopic state

observations is included. Note that this information can be both qualitative and quantitative, so this approach does not provide an entirely quantified measure of complexity.

A number of measures have been proposed to calculate the complexity of a system in numerical terms. However, the usefulness of such measures is not always clear, and greatly depends on the user understanding exactly both what is being measured and how the measure should be used (Feldman and Crutchfield, 1998). Indeed, one review of such measures finds that the best measure "can be used in practice to infer the presence of a complex system" (Ladyman et al., 2013, p.24). I suspect that one would already know the system was complex without calculating the Statistical Complexity. Hence, introducing numerical measures of complexity may actually increase ambiguity, rather than clarity. Complex systems in this study are therefore determined using the qualitative concepts of emergence and the four properties of complexity as outlined above. The depth of information required to describe the system is found using Bar-Yam's approach applied in the context of the problem.

2.3. Complex Problems

You do not have to read further than the title of "Complex problem solving: a field in search of a definition?" (Queseda et al., 2005) to interpret that, as with the term *complex system*, no single definition of a complex problem exists. Fortunately, however, it is generally agreed that problems involving complex systems are complex problems (Funke, 2012; Fischer et al., 2012), so there need not be another five pages exploring characterisations. Three of the five features of complex problems differentiated by Funke (2012) – complexity, connectivity and dynamics - map directly onto the properties of complex systems discussed previously. These are defined in Table 2.

Table 2: How the features of complex problems relate to the properties of complex systems

Feature	Complexity	Connectivity	Dynamics
Definition (Funke, 2012)	The problem situation contains a high number of variables	A high number of these variables are interconnected	The problem system can change over time without intervention, and may give rise to unexpected behaviours when interfered with
Emergence			x
1. Ensemble of Many Elements	x		
2. Interactions		x	
3. Disorder			x
4. Robust Order and Memory			x

The remaining two features, termed intransparency and polytely, are concerned with the problem itself and indicate why complex problem solving is so challenging. Intrasparency refers to the lack of clarity in problem formulation, regarding both the variables which should be involved and the definition of the goal. Polytely comes from the Greek roots *poly* and *tel*, meaning many goals. In a complex problem, there may be multiple goals to reach, which can also conflict with each other, requiring prioritization of the goals or compromises.

Generally speaking, approaches to solve complex problems comprise two main stages known as *knowledge acquisition* and *knowledge application,* (Fischer et al., 2012; Greiff et al., 2015). The procedures, tools and techniques to acquire and apply knowledge differ depending on the system being explored and the goals to be reached.

2.3.1 Knowledge Acquisition

"At first, the problem solver has to acquire knowledge about the problem" (Greiff et al., 2015, p.36). After reviewing the literature, I have split this knowledge acquisition stage into three aspects: knowledge of the problem itself; knowledge of the system and knowledge of experimental design.

2.3.1.1 Knowledge of the Problem

First, the solver must clearly define the system the problem is concerned with as well as the goal or goals to be reached. This can be thought of as the problem formulation process, in which a system representation is created, containing only the real-world areas of interest pertinent to the problem (Kasser and Palmer, 2005). The most complete process found in the literature for creating a System of Interest (SOI) is outlined in Kasser (2015). This process consists of 8 activities which "should be performed in an iterative sequential parallel manner" (Kasser, 2015, p.3). These activities are:

1. **Examine the problem situation from several perspectives**

Multiple perspectives allow for a better, less likely to be erroneous, understanding of the problem situation than a single perspective. A good approach is to ask 'who', 'what', 'where', 'when', 'why' and 'how', which intuitively cover a range of holistic thinking perspectives. These perspectives are formalised in Kasser (2013).

2. Develop an understanding of the problem situation

The solver is aiming to understand:

- The stakeholders involved in the problem situation;

- The basic behaviours of the SOI;

- The nature of the problem: whether this is how the system is structured, what operations the system performs, or whether the functions that support these operations do so appropriately?

3. "Create the Feasible Conceptual Future Desirable Situation (FCFDS) containing the SOI" (Kasser, 2015, p.3)

An important part of understanding and solving the problem is deciding what a successful outcome looks like. For example, a shop might have a concept of a future desirable situation where sales are boosted by 300%, but is this feasible? That really depends on the current situation and the tools (or solutions) the shop can implement to boost sales. When you consider the aspect of feasibility, the FCFDS becomes more than just a concept, and rather more like a solution set. According to Kasser and Zhao (2016), the FCFDS should be studied to ensure that it is:

a) **operationally feasible**: the solutions or combinations of solutions included are achievable;

b) **structurally feasible**: suitable technologies exist at the appropriate Technology Readiness Levels[3];

c) **quantitatively feasibl**e: cost, risk and uncertainties are at acceptable levels;

d) **t**e**mporally feasible**: that it will be ready when needed.

4. Use the principle of hierarchies

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[3] Technology Readiness Levels in this work are taken as defined by the European Commission in the Horizon 2020 work programmes (EC, 2016, p.29).

Many complex systems could be defined as 'systems of systems', which is a term widely used in the field of systems engineering. These are "large-scale integrated systems which are heterogeneous and independently operable on their own, but are networked for a common goal" (Jamshidi, 2008, p.44 cited in Evans, 2016, p4). 'Systems of systems' will henceforth be referred to as *systems of subsystems*, to differentiate between the SOI (the system) and the systems that are comprised within it (the subsystems). This idea relates directly back to the 'ensemble of many elements' property of complexity. When formulating the problem, it is beneficial to consider whether the SOI is formed of subsystems, and at which level these need to be described. Consider that the subsystem of a SOI may become the SOI in another problem situation.

5. Abstract out the parts of the situation that are not pertinent to the problem

This is most easily understood by example. Kasser (2015, p. 8) provides the following:

> *"Consider the problem of docking a resupply vehicle such as the US Space Transportation System (Space Shuttle) to the International Space Station (ISS). Each is a complex system in itself, yet when solving the problem of docking a Shuttle to the ISS, all the underlying complexity that is not relevant to the docking problem is abstracted out. Thus, we construct a closed system view to simplify the problem by abstracting out (filtering out) everything other than information pertinent to the: relative positions of the spacecraft; relative velocities of the spacecraft; relative orientation in X, Y and Z axes of rotation."*

6. Partition the FCFDS (solution set) into the SOI and adjacent systems

A possible solution included in the FCFDS for the shop scenario might be to expand and open a new branch. If the original shop was defined as the SOI, then this solution is obviously outside of the existing boundaries of that system. This activity therefore encourages the solver to consider the boundaries of the original SOI and to partition the solution set into those that apply within its bounds and those that concern adjacent systems.

7. Optimise the interfaces

Wymore (1997) shows that contrary to "conventional systems engineering wisdom," it is possible to optimise a system by individually optimising its subsystems. However, this relies on the interfaces between the subsystems being properly defined and is a crucial consideration for the final activity, in which the subsystems are formally created.

8. Partition the SOI into subsystems

2.3.1.2 Knowledge of the System

Once the system and subsystems have been defined, knowledge of the system is gained by exploring the system behaviour in more detail. Fischer et al. (2012) categorise this into *instance knowledge* and *structural knowledge*. Instance knowledge is information regarding the system's state in relation to actions taken, i.e., when '*x*' action is taken, '*y*' happens to the system state. For example, when the red button is pushed, the missile is launched. Based on this instance knowledge, the solver can infer structural knowledge about the relationships between subsystems (e.g., the red button must be connected to the missile launcher).

This instance and structural knowledge is used by the solver to determine the most important elements and relationships within the problem scenario. This may lead to changes in the system representation assumed in the problem formulation process. The ultimate aim of the exploration stage is to gain sufficient knowledge of the problem situation, in order that the solver may use it to derive a solution in the knowledge application stage (Greiff et al., 2012).

Exploration is done by developing hypotheses, designing and conducting experiments on the problem scenario and drawing conclusions from the experimental results. There are a number of processes involved in this which fall into the four spaces of the framework developed by Schunn and Klahr (1995). These spaces in the context of complex problem solving are the:

1. **Hypothesis space**: hypotheses about the causal relationships within the system are formed, based on the current representation of the SOI;

2. **Data representation space**: representations of the relevant system elements within the hypothesis are chosen and a model of the system is developed;

3. **Experimental paradigm space**: a suitable class of experiments is chosen based on the hypotheses;

4. **Experiment space:** the system parameters within the chosen class of experiments are set.

Gaining knowledge of the system therefore requires knowledge of appropriate experimental designs for the given system, which I consider as the final aspect of knowledge acquisition.

2.3.1.3 Knowledge of Experimental Design

A good experiment achieves three things: it acquires information relevant to the hypothesis; provides easily-interpreted and unambiguous results and minimises the costs and risks associated with conducting experiments (Schunn and Klahr, 1995). If the experiment does not provide interpretable and relevant results the solver risks wasting money and time; as well as mental, physical and computational effort, and facing further consequences of these costs. The experimental design stage is therefore critical when solving complex problems.

Once a hypothesis has been formed, the foundation of any experiment is a model of the system being studied. The variation of this model, either its inputs or its structure or both, forms the experiment, and the results are the observed outcomes of these variations. Fisher (1971) illustrates the principles of experimentation using the following hypothesis – "A lady declares that by tasting a cup of tea made with milk she can discriminate whether the milk or the tea infusion was first added to the cup" (p. 11). The model in this case is a cup of tea, which is varied in structure according to whether the tea or milk is added to the cup first. As systems become more complex, so do the models which are created to represent them. The majority of experiments concerning complex systems rely on numerical computer simulations to model the system. However, before experiments can be conducted to explore the system behaviour, the simulation itself must be validated to ensure it is an accurate representation of the system (Min et al., 2010).

Sensitivity Analysis (SA) is commonly used to gain an understanding of simulated problem scenarios (Kleijnen et al, 2005). The simplest sensitivity experiments are one-factor-at-a-time (OFAT) experiments, in which, as the name suggests, a single factor is varied whilst all other variables remain constant. The term 'factor' is used in the Design of Experiments (DOE) to refer to the inputs of interest, which are changed during the experiments. Although OFAT experiments provide unambiguous results, they are unsuitable for complex systems. Analysing a single factor at a time in a system containing many elements would not only be computationally expensive, but does not allow the interactions between factors to be observed (Kleijnen et al., 2005). Interactions give rise to emergent behaviours, which are part of the

knowledge of the system that the solver is trying to gain in the knowledge acquisition stage. For this reason, local methods, which again only vary one factor at a time and typically within one point of the factors' space, are unsuitable (Saltelli et al., 2004). Regression analysis also tends to perform poorly for complex systems (Nguyen and Reiter, 2015). This is because it attempts to describe the output in terms of a linear combination of the input factors when, in reality, the relationship between input and outputs for complex systems is rarely linear.

Based on the problems described above, we can determine that SA techniques for complex systems must be able to:

1. Explore the entirety of the factors' input space;

2. Evaluate the interactions between factors;

3. Cope with non-linear and non-monotonic relationships between factors.

Both variance-based methods and screening methods meet these criteria. Variance-based methods are able to give quantitative results, indicating how much more important one factor is than another, whereas screening methods can be considered qualitative, only giving the ranking of factors and not the relative importance (Saltelli et al, 2004). However, screening methods have a significantly reduced computational cost, making them desirable for conducting SA of models with a large number of input factors or long execution time.

2.3.2 Knowledge Application

Once knowledge of the problem, system and appropriate experimental design has been gained, this knowledge is combined and applied to the problem scenario. In this stage, the solver moves through DOE, to conducting the experiments and then analysing the results. This in turn helps the solver to better understand the problem, system and experimental design, meaning knowledge acquisition and application are cyclical stages. Based on the outcome of the analysis, the solver may choose to revise the model, redesign the experiments, or implement a solution or combination of solutions.

In order for the appropriate action to be taken, it is crucial that the solver gains as much information as possible from the experiments and interprets this information correctly. This not only requires a solid understanding of the sensitivity measures which can be calculated

from the method once implemented, but also of appropriate data representation techniques which allow the trends of these measures to be identified.

Once a set of solutions has been determined from the experimental results, the optimal solution or combination of solutions can be determined using a variety of optimisation techniques. The crucial aspect of any optimisation is the creation of the objective function, which defines the criteria that solutions must satisfy, using equality and inequality constraints. The optimal solution is that which satisfies all of the constraints, and has either the minimum or maximum objective value, depending on the function design (Zhao, 2013).

2.4. Summary

In this chapter, a definition of complex systems has been introduced, based on the characteristics of emergence and complexity. The two stage approach to problem solving has been discussed in the context of complex systems. It has been demonstrated that the primary stage of knowledge acquisition can be separated into three distinct categories: knowledge of the problem, knowledge of the system and knowledge of experimental design. Before experiments are conducted in the knowledge application stage, it is crucial that the solver understands the experimental techniques appropriate for the problem. Variance-based and screening methods of Sensitivity Analysis (SA) are introduced as being particularly suited for determining the critical factors for complex systems which can be modelled using computer simulation. As the experimental results from these analyses will be used to inform the next action to be taken, the importance of data representation is also stressed. The next chapter covers appropriate SA methods, their sensitivity measures and how quantitative multivariate data can be analysed to determine trends across and within the subsystems of complex systems.

Chapter Three

Generating and Analysing Complex System Data

"Conducting data analysis is like drinking a fine wine. It is important to swirl and sniff the wine, to unpack the complex bouquet and to appreciate the experience. Gulping the wine doesn't work."

D.B. Wright (2003)

3.1. Introduction

This chapter focusses on the second objective of this thesis, which is 'to determine appropriate experimentation and data visualisation methods for complex systems'. It is crucial that not only is as much information about the system behaviour gathered through experimentation, but that this information is analysed efficiently and comprehensively to gain a thorough understanding of the underlying causes of this behaviour, i.e., the critical factors of the system. As previously discussed, variance-based and screening sensitivity analyses are well suited for exploring the results of complex system simulations. One technique of each type is described in detail, and then a range of methods for data visualisation and analysis are introduced.

The italicised content in Section 2.1 has been taken from Douglas et al., 2016a, in accordance with the ICE publishing agreement in Appendix B.

3.2. Sensitivity Analysis Methods

In order to solve problems concerning complex systems, the system behaviours must be known. Sensitivity Analysis (SA) refers to a group of techniques used to determine how changes in the input factors of a model affect the model outputs. Therefore they can be used to explore system behaviour. Depending on how the input factors are varied and the sensitivity measures calculated, SA can be used to investigate three things (Saltelli and Sobol, 1996):

1. **The active factors**

Referred to as screening methods, these techniques are loosely based on one-factor-at-a-time (OFAT) experiments but allow interactions between factors to be assessed through the overall experimental design. As with OFAT experiments the value of each input factor is varied and the output observed, in order to determine the effect of each factor. However, this variation and observation is repeated whilst the other factors take different values in order to assess the interactions between them. Input factors are typically varied between low to high values within the search space and the main effects and interaction effects calculated (Cotter, 1979). These methods are used on models with high numbers of factors and identify those which are active. This allows the model to be simplified by the removal of inactive factors (Campolongo et al., 2007).

2. The parameter effects on the model

These methods vary the input factors from a base data point and are considered local methods (Saltelli and Annoni, 2010). As previously mentioned, local methods are not suitable for complex systems as they do not allow the solver to observe the interactions between factors, which are crucial for understanding emergent behaviour. Local methods are therefore not discussed in this chapter.

3. The contribution of factors to output uncertainty

These methods vary the input factors across the whole search space, rather than around a single point and are referred to as global methods. Input factors take discrete values across the whole search space (rather than low and high values as with screening methods). This greater level of detail allows the differences in the importance of factors to be quantified. Global approaches include regression and variance-based methods. However, only variance-based approaches are discussed in this chapter, due to the unsuitability of regression for non-linear models.

3.2.1 Screening Methods

Although a number of different screening methods exist (Cotter, 1979; Andres and Hajas 1993), the Morris method is the most widely used. This is no doubt because it is "the most appealing for a range of problem settings" (Saltelli et al., 2004, p.92). The original method and several variations are discussed in this section.

The Morris Method

The Morris Method (Morris, 1991) is an effective screening method for models with large numbers of factors or high computational cost. In a comparison of SA methods for models of buildings, it was found to be acceptable for determining sensitivity and interactions when compared with variance-based methods (Nguyen and Reiter, 2015). *It uses the data from randomised OFAT experiments to calculate Elementary Effects (EE), which are each attributable to one input factor. Sensitivity information is then calculated using the EE.* Although the EE are technically local sensitivity measures, a suitable random sampling strategy can ensure coverage of the search space, overcoming the drawbacks of local analyses (Ruano et al., 2012).

This method assumes the search space is a k-dimensional, p-level grid, where k is the number of model factors, and p the number of levels that each input factor, X_i varies across. All factors are uniformly distributed, taking discrete values between [0, 1] and then transformed to their real distributions (Campolongo et al., 2007).

*From a starting point **X**, the EE for the ith factor is found by evaluating the change in the output, **Y**, when this factor is increased or decreased by Δ, over Δ.*

$$EE_i = \frac{Y(X_1, \dots, X_i \pm \Delta, \dots X_k) \pm Y(X_1, \dots, X_k)}{\Delta}$$

*It is recommended that Δ takes the value of $p/[2(p-1)]$, where p is an even number, to ensure symmetric treatment of outputs and economical design. **X** can take any value within the search space; provided that it is still within the search space after the addition or subtraction of Δ. Trajectories of (k+1) points are constructed by randomly selecting a starting point, and moving OFAT, by the addition or subtraction of Δ, in a random order.* Two example trajectories are shown in Figure 1. The black circles indicate the starting position of each factor, which are then moved by Δ in a random order as shown in the legend. In this way the input factors are varied between a range of low and high values covering the search space.

From r random trajectories, giving a total of 2r(k+1) simulation runs, two sensitivity measures for each factor are calculated using the EE as follows:

$$\mu_i = \frac{\sum_{i=1}^{r} EE_i}{r}$$

$$\sigma_i = \sqrt{\frac{\sum_{i=1}^{r}(EE_i - \mu_i)^2}{r}}$$
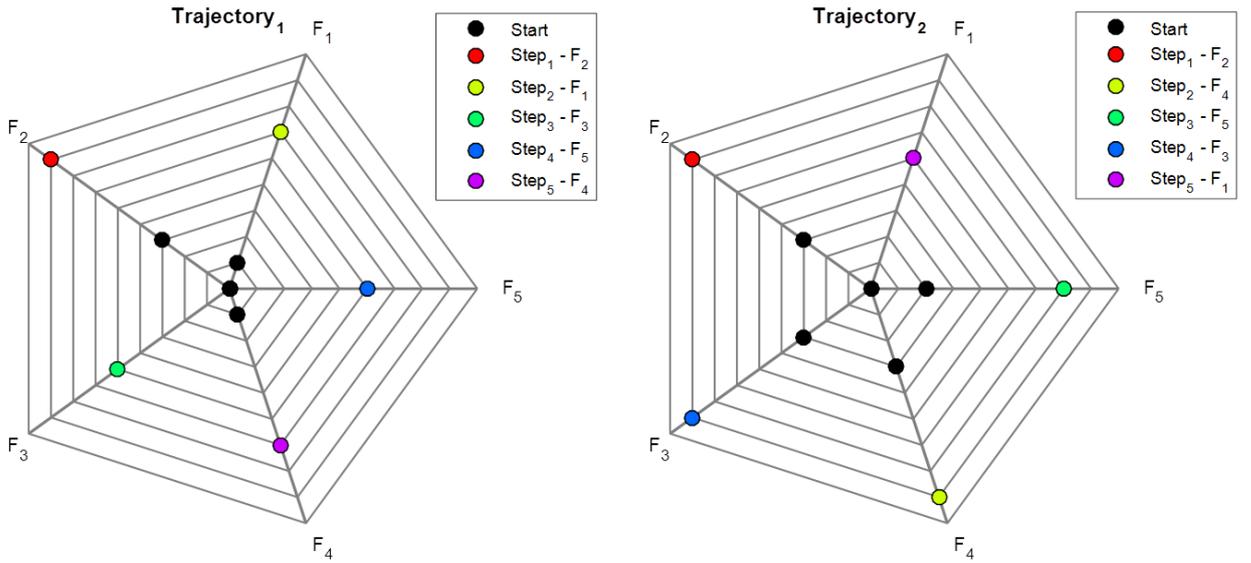
Figure 1: Two different Morris trajectories for a model with k = 5 factors and p = 10 levels (Douglas et al., 2016a)

The mean value for each factor, μ$_i$, indicates the first order, linear effect of the factor on the output. However, for non-monotonic models it is possible that opposite signs of EE will cause low μ values for important factors. The improved measure, μ^*, was therefore introduced by Campolongo et al. (2007), which uses the absolute values of the EE, to eliminate this error. The value of μ^* can be used to rank the factors in order of importance (Campolongo et al., 2011). *The standard deviation, σ$_i$, indicates non-linear effects due to interactions between factors.* When both the μ^* and σ values are considered, the effects of the factor can be categorised as shown in Table 3 (Santiago et al., 2010). Although all factors with a high σ value have interactions with other input parameters (Sanchez et al., 2014), those with a low μ^* value can be considered negligible because these interactions do not impact the model.

Table 3: The categorisation of factor effects for Morris based on μ* and σ values

	Low μ*	High μ*
Low σ	Negligible	Linear and Additive
High σ		Nonlinear or Interaction

The choice of sampling strategy used to generate trajectories is important because ineffective sampling may lead to inadequate coverage of the search space, giving erroneous results. The original method (Morris, 1991) suggests that the total number of simulation runs should be of the same order of magnitude as the number of inputs, as opposed to fractional factorial plans where the number of runs is of the order of k^2. Morris' example has 20 inputs and only evaluates 4 trajectories, leading to 84 simulation runs. However this approach provides only limited information and, as such, the number of trajectories is considered too low by Campolongo et al. (2007). In their work, they first evaluate 4 inputs using 20 trajectories (200 simulation runs), and then recommend a new sampling strategy to ensure even better coverage. They recommend generating a high number of trajectories (r = 500-1000) and selecting a smaller group (e.g. r =10) with the largest spread, as determined by a distance function. However, as the calculation of distance requires a time-consuming brute force evaluation, it is only worthwhile taking this approach if the model takes a significant time to run. Otherwise, all of the generated trajectories may as well be evaluated. Other sampling strategies which have been explored are the cell-based strategy (Saltelli et al., 2008), which was found to be no better than the previous strategy, and a radial OFAT design (Campolongo et al., 2011).

3.2.2 Variance-based Methods

Variance-based methods, which apportion the output variance to the variance in the input factors, are often used as a benchmark when comparing or developing SA methods because they are considered to give reliable and consistent results when ranking factors (Campolongo et al., 2007; Nguyen and Reiter, 2015). Both the Sobol and Fourier Amplitude Sensitivity Test (FAST) methods are widely cited in the literature of variance-based and global SA (Chan et al., 1997; Nguyen and Reiter, 2015; Saltelli et al., 2010).

FAST is able to compute the main effect (first order effect) of a factor, but cannot easily calculate the higher order effects arising due to interactions (Saltelli and Bolado, 1998). However, it is likely that within a complex system, interactions will account for a non-

negligible portion of the sensitivity. It is for this reason that Sobol is preferred, as it allows not only the first order effect to be calculated but also the Total Sensitivity Index (TSI), which incorporates the first order effects measure and the effect of all other factor interactions.

Sobol Method

The Sobol method (Sobol, 2001) uses Monte Carlo samples to explore the input factor space and to calculate the first order effects and TSIs. In a model with three factors, a, b and c, the TSI for factor a would be calculated as follows (Chan et al., 1997):

$$TSI_a = S_a + S_{ab} + S_{ac} + S_{abc}$$

where S_a is the sensitivity index for parameter a (the first order effect), S_{ab} is an example of a second order sensitivity index, and S_{abc} is the only third order sensitivity index. This is easily extended: for the ith factor in a model with k factors, the TSI would be calculated as (Dimov and Georgieva, 2010):

$$TSI_i = S_i + \sum_{l_1 \neq i} S_{il_1} + \sum_{l_1, l_2 \neq i, l_1 < l_2} S_{il_1 l_2} + \cdots + S_{il_1, \ldots, l_{k-1}}$$

The TSI takes a value between 0 and 1 which indicates the importance of each factor. Importance is classified as shown in Table 4 (Chan et al., 1997).

Table 4:Classification of factor importance for variance-based methods based on TSI value

TSI value	Importance
TSI ≥ 0.8	Very important
0.5 ≤ TSI < 0.8	Important
0.3 ≤ TSI < 0.5	Unimportant
TSI < 0.3	Irrelevant

Given a model of the form $Y = f(X_1, X_2, \ldots, X_k)$, the sensitivity indices are calculated from the output variance, which is the sum of the variances for each of the k factors and all combinations of factors (Campolongo et al., 2007).

$$V(Y) = \sum_i V_i + \sum_i \sum_{j>i} V_{ij} + \ldots + V_{12\ldots k}$$

The sensitivity index for factor i is calculated by:

$$S_i = \frac{V_{X_i}(E_{X_{\sim 1}}(Y|X_i))}{V(Y)}$$

$E_{X_{\sim 1}}(Y|X_i)$ denotes the mean value of Y, which is calculated using an input matrix of all factors except X_i, which remains constant. V_{X_i} is then the variance of the mean for all values of X_i. The TSI for i is given by:

$$TSI_i = 1 - \frac{V_{X_{\sim i}}(E_{X_i}(Y|X_{\sim i}))}{V(Y)}$$

A number of estimators for S_i and TSI$_i$ have been suggested which relate to the sampling process: in this section those used by Saltelli et al. (2010) are described for the radial sampling method, which was found to be best practice. Note that the estimator for S_i is first introduced by Jansen (1999).

To complete the analysis, two independent sampling matrices are required, **A** and **B**. The columns of the matrices vary from 1 to k, and the rows from 1 to N, where N is the sample size of the Monte Carlo estimate. The matrices **A** and **B** are generated from Sobol's quasi-random sequences (Sobol, 1976) of size (N, 2k) where **A** is the left half of the sequence and **B** the right half. Though called quasi-random, these sequences are not random at all. Samples of X_1 to X_k are generated over the input factor space and, as N increases, samples are taken from previously un-sampled space.

In the radial sampling method, the analysis is split into N blocks of (k+1) samples, where each block produces one TSI for each factor, which is calculated as follows:

$$TSI_i = \frac{1}{2N}\sum_{j=1}^{N}(f(A)_j - f(A_B^{(i)})_j)^2$$

For block N, $\mathbf{A_B}^{(i)}$ represents a set of input factors which are taken from row N of **A** for all factors other than i. The ith factor is substituted with the factor value from row N of **B**. The final estimates of the TSI and S$_i$ are found by averaging the N estimates.

If only the TSI for each factor is calculated, the total cost of the experiment is $N(k + 1)$. However, calculating the value of S_i requires the evaluation of the function using **B**, which increases the cost to $N(k + 2)$:

$$S_i = 1 - V(Y) - \frac{1}{N} \sum_{j=1}^{N} f(B)_j (f(A_B^{(i)})_j - f(A)_j)$$

This is a non-trivial addition considering that N is recommended to take values greater than 500 (Saltelli et al., 2010).

3.3. Data Interpretation

For complex systems it is unlikely that the solver will perform a single SA to explore the whole system at once. This would not only be very difficult to formulate and time consuming to conduct, but also would not necessarily provide a useful or comprehensive understanding of the system. Much greater insight into the system behaviour and appropriate model refinements or experiments can be gained by exploring each subsystem separately and then analysing the trends between subsystems. Data interpretation must therefore be done at two levels: at subsystem level to find the most important factors and factor relationships for the given subsystem; and then at system level to understand the trends between these subsystem results.

Efficient and comprehensive interpretation of the data usually requires it to be transformed to an appropriate visual representation. This can be done by directly plotting the data using simple graphical methods such as bar charts, line graphs and scatter plots, or matrices of these plots. However, as the dimensionality of the data increases, more sophisticated visualisation techniques may be more suitable (Keim, 2002).

Alternatively, the data trends can be summarised by applying Multivariate Analysis (MA) methods, and then these trends visualised. MA techniques are used to determine the relationships in 'multivariate' datasets, which contain observations of multiple variables for a number of different individuals (Chatfield and Collins, 1980). MA methods are suitable for analysing the trends both within and between subsystems, depending on how the individuals and variables are defined, for example:

- Within a subsystem, different simulation runs could be considered as individuals and the system outputs whose sensitivity is tested as the variables. This relates directly back to the nature of complex problems, which often have multiple goals

- When analysing trends between subsystems, the subsystems could be considered as the individual, and the sensitivity measures for each factor as the variables

3.3.1 Visualisation Techniques

The different visualisation and MA techniques are illustrated using Fisher's Iris Flower dataset (1936). The dataset contains the values of 4 variables (sepal length, sepal width, petal length, and petal width) for 50 individuals each of 3 different Iris species. As one of the species is linearly separate but the other two overlap, it is a good test for data analysis and visualisation techniques, particularly those using machine learning (Swain et al., 2012). It is commonly used to illustrate visualisation and MA techniques (examples include Alsakran et al., 2016; Grinstein et al., 2001; Wagstaff et al., 2001). The data is included in Appendix C. All graphs were generated by the author.

3.3.1.1 Heat and Height Maps

Heat maps are an array of cells which are coloured based on some data value or function, and particularly useful for comparing similar elements and identifying trends (Barrow et al., 2009). Height maps are similar, except that the cells are given a height related to the data value or function instead (Grinstein et al., 2001). The colour is also based on this value, so colour corresponds to height, not a secondary variable. Figure 2 shows heat and height maps of the Iris data, which has been ordered by species.
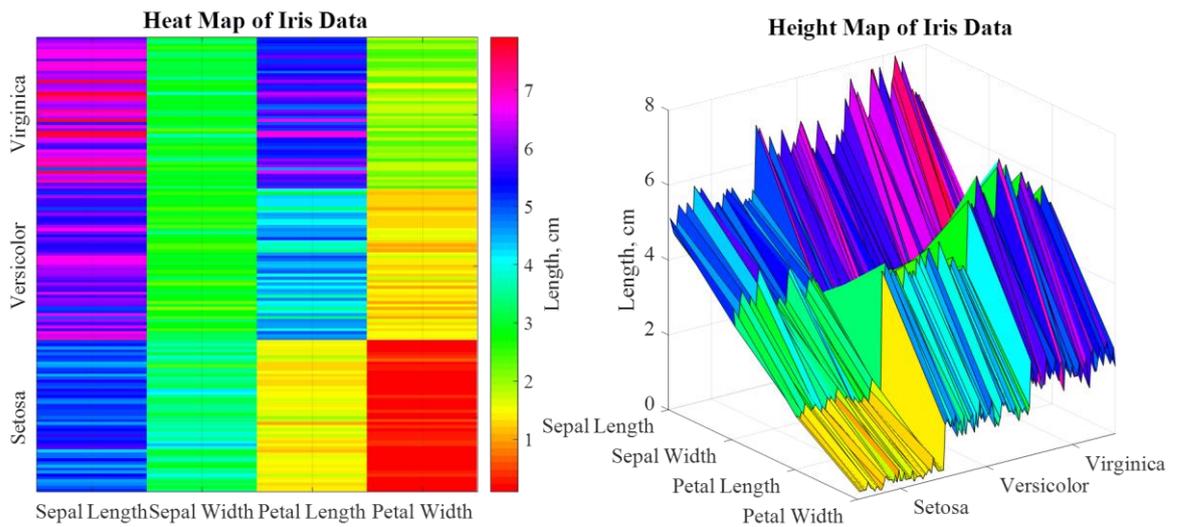
Figure 2: Heat and height maps for Iris data, ordered by species

3.3.1.2 Parallel Coordinates
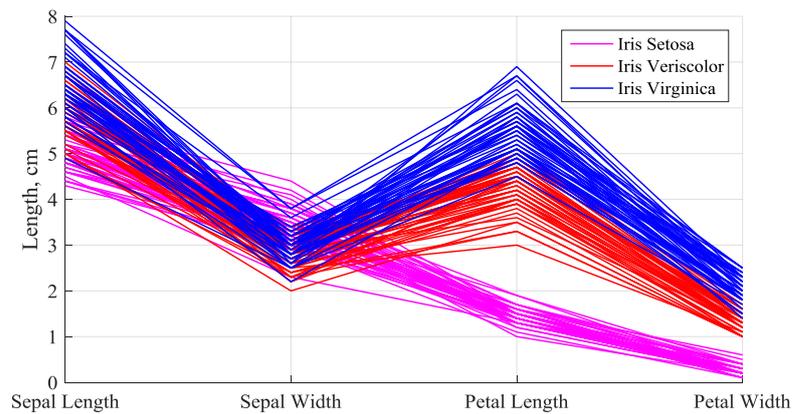
Figure 3: Parallel Coordinates of Iris data, grouped by species

In Parallel Coordinates each data point is mapped onto N evenly-spaced vertical axes of a 2-dimensional image allowing the N-dimensional hypersurface to be studied, where N is the number of observed variables (Inselberg and Dimsdale, 1990). The data points for each individual are connected, creating a so-called polyline which crosses all of the axes at the positions relating to the values for each dimension (Fua et al., 1999). Figure 3 shows parallel coordinates for the Iris dataset, grouped by species. This representation allows similar polylines to be identified. However, as the number of observations increases it becomes more and more difficult to identify groups (Artero et al., 2004). This can be mitigated by applying

various clustering techniques which condense the displayed data and improve the visual layout (Fua et al., 1999; Artero et al., 2004; Alsakran et al., 2016).

3.3.1.3 Dimension Stacking

In Dimension Stacking *N*-dimensional data is displayed in a 2D format by stacking pairs of dimensions, which are broken down into sections based on the cardinality of the dimension (LeBlanc et al., 1990). Each dimension should have no more than 4 or 5 categories, and if continuous, data should be discretised (Hoffman and Grinstein, 2001). The Iris Data can be thought of as having 4 dimensions each of cardinality 3, when the continuous length data is split into 3 equal categories covering the range of each variable. The two outer dimensions form a 3x3 grid, each cell of which is split into another 3x3 grid representing the two inner dimensions. Values in the N-dimensional space are mapped onto the 2D image by calculating their index in each dimension. This representation is shown in Figure 4.
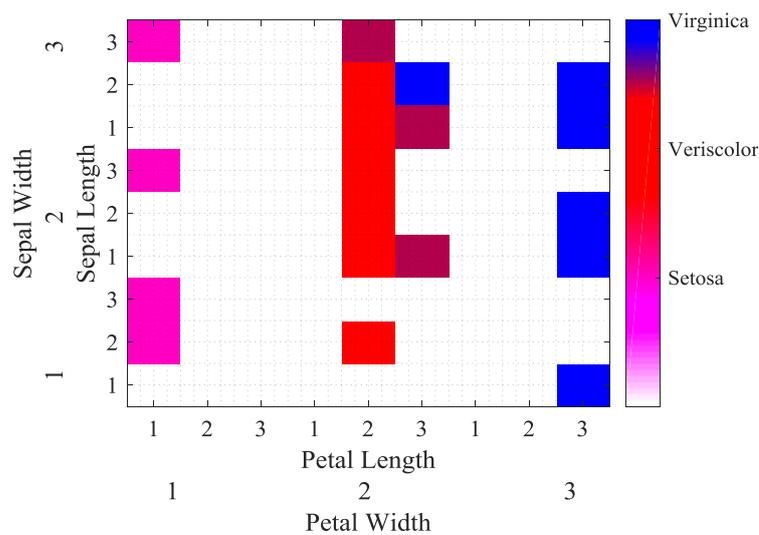
Figure 4: Dimension Stack of Iris data, grouped by species

3.3.1.4 Star Glyphs

Glyphs are icons which are used to represent the individuals of a dataset, and are created by mapping the N-dimensions of the data to a visual attribute of the icon such as shape, colour, texture or size (Borgo et al., 2013). Star glyphs are commonly used (Hoffman and Grinstein, 2001), which are very similar to radar plots. They are formed of *N* equally spaced lines extending outwards from an origin, whose lengths relate to the value of the data in each dimension, connected to form a polygon. The data in each dimension is scaled independently

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so that the origin represents the minimum value and the end of the line represents the maximum. Figure 5 shows star glyphs representing the average of the Iris data for each species.

Setosa   Veriscolor   Virginica
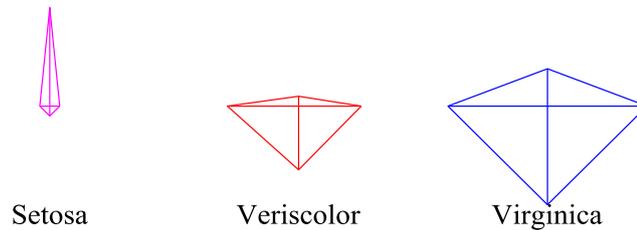
Figure 5: Star Glyph representation of Iris data (average), grouped by species

3.3.2 Visualisation Techniques Used

The visualisation techniques taken forward for the rail application study are heat and height maps, which are used as tools to understand the whole system results (Section 6.4). Parallel coordinates and star glyphs were not deemed suitable for the subsystem analyses due to the large number of individuals in the dataset (3,920). They were also not used for the overall system analysis as they relate to the values of variables, rather than rankings. Dimension stacking was not used as I do not feel it represents information in a way that is intuitive to the reader.

3.3.3 Multivariate Analysis

Contrary to the visualisation techniques introduced in the previous section, which simply represent the dataset and rely on the solver to identify the trends, MA techniques analyse the data to find the underlying trends so that they can be represented. This is particularly of use for highly dimensional data in which patterns are hard to identify (Clark and Ma'ayan, 2011).

3.3.3.1 Principal Components Analysis

Principal Components Analysis (PCA) was developed by Pearson (1901), and is "often considered as the basic method of factor analysis" (Saporta and Niang, 2009, p.1). It is a dimension reduction method that creates new, independent variables, using linear combinations of the original variables, to describe the variation in the data (Clark and Ma'ayan, 2011). The Principal Components (PCs) are defined so that the first accounts for the

most variability in the data, the second for the next greatest variability in an orthogonal direction, and so on. Briefly, the steps to calculate the PCs are as follows (Smith, 2002):

1. **Normalise the data**

The data should be standardized to ensure their contributions to variance are comparable, by rescaling each variable to have unit variance. If the data is recorded rather than generated, missing values and outliers should be replaced (Groth et al., 2013).

2. **Calculate the covariance matrix**

Covariance is a measure of how much a variable varies with respect to another variable, and is calculated for *n* individuals between two dimensions (A and B) as follows, where μ represents the mean:

$$cov(A, B) = \frac{\sum_{i=1}^{n}(A_i - \mu_A)(B_i - \mu_B)}{(n - 1)}$$

The covariance matrix shows the covariance of every variable with every other variable. The diagonal of the matrix shows the variance of each dimension, i.e. its covariance with itself. For a 3 dimensional dataset the covariance matrix would be:

$$C = \begin{pmatrix} cov(A, A) & cov(A, B) & cov(A, C) \\ cov(B, A) & cov(B, B) & cov(B, C) \\ cov(C, A) & cov(C, B) & cov(C, C) \end{pmatrix}$$

3. **Calculate the eigenvectors and eigenvalues of the covariance matrix**

4. **Order Principal Components**

The Principal Components (PCs) directly relate to the eigenvalues of the covariance matrix. The highest eigenvalue is the first PC.

5. **Identify correlation between variables and PCs**

Once the PCs have been found, the solver needs to interpret the trends they signify. This is done by investigating the correlation between the original variables and the PC, where a correlation value can be specified to indicate significance (Roths, 2016). Scatter plots,

using the PC as axes, are often used to understand the relationship between individuals in the dataset and the trends.

PCA using the Iris dataset identifies two PCs that account for 95% of the variability in the data. Using the results in Table 5 and a correlation value of 0.5 to indicate significance, it can be deduced that the primary trend is for Sepal Length, Petal Length and Petal Width to increase together. The second PC2 only increases with one variable, Sepal Width. Figure 6 indicates that the Setosa species has shorter sepals and shorter and thinner petals than the Veriscolor and Virginica species, and that all species have a range of sepal widths.

Table 5: Principal Components of the Iris data individuals

Variable	PC1	PC2
Sepal Length	0.52	0.38
Sepal Width	-0.27	0.92
Petal Length	0.58	0.02
Petal Width	0.56	0.07
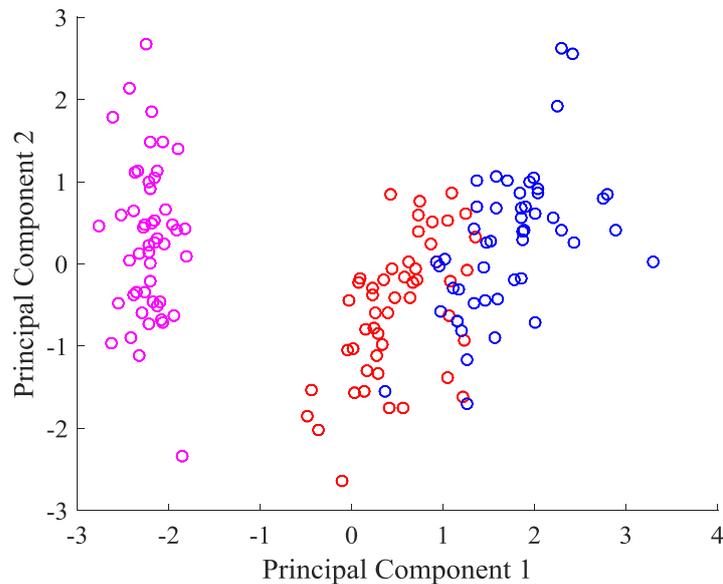
Figure 6: Iris data individuals plotted in relation to Principal Components

3.3.3.2 Cluster Analysis

Cluster analysis, or clustering, is another form of data reduction which organises the dataset individuals into classes of similar individuals based on their closeness (Nadif and Govaert,

2009). Closeness is determined using a distance calculation: typically the Euclidean distance between two vectors:

$$d(X,Y) = \sqrt{\sum_{i=1}^{k}(X_i - Y_i)^2}$$

Clustering can be done using hierarchical or partitional clustering approaches, the most common of which are Ward's method (Ward, 1963), and the k-means algorithm respectively (Govaert, 2009). As with PCA, it is important to rescale the data before clustering to ensure variables with large variances do not dominate.

Ward's Method

The method suggested by Ward is an agglomerative hierarchical method, meaning that it starts with all individuals as clusters, and iteratively merges the closest clusters based on an *agglomerative criterion* until there is a single cluster (Nadif and Govaert, 2009). The criterion for merging in this case is the minimum error sum of squares, which is calculated as follows for a group of *n* individuals:

$$ESS = \sum_{i=1}^{n} x_i^2 - \frac{1}{n}\left(\sum_{i=1}^{n} x_i\right)^2$$

Figure 7 is a dendrogram of the Iris data, showing the clustering hierarchy. Three distinct clusters have been highlighted. The Setosa species makes up the single branch cluster, and the other two contain both Veriscolor and Virginica species individuals.
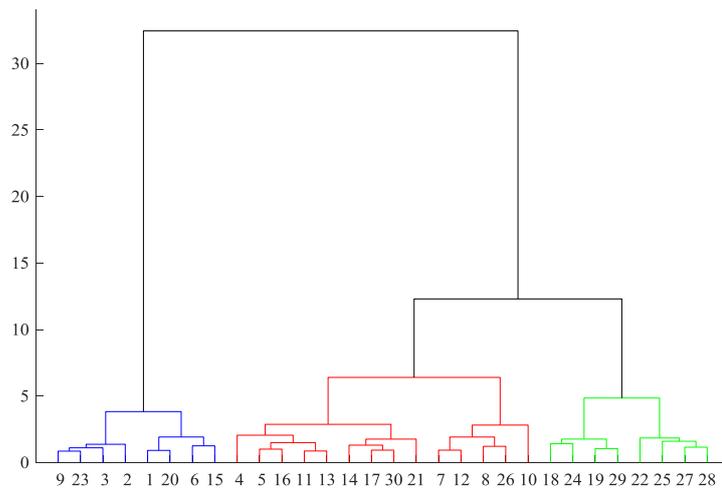
Figure 7: Dendrogram of Iris data clustered using Ward's method

K-means Algorithm

There is no hierarchy to k-means clustering. Instead, the dataset individuals are partitioned into *k* clusters based on their closeness to *k* randomly selected cluster centres. After each inclusion of another individual, the cluster centre is updated so it reflects the mean of its assigned individuals (Macqueen, 1967). The difficulty in k-means is selecting the optimal value of *k,* although the utilization of background information can help (Wagstaff et al., 2001). Figure 8 shows the Iris data clustered into 3 groups using k-means, using petal length and width as axes. The black circles indicate the cluster centres.
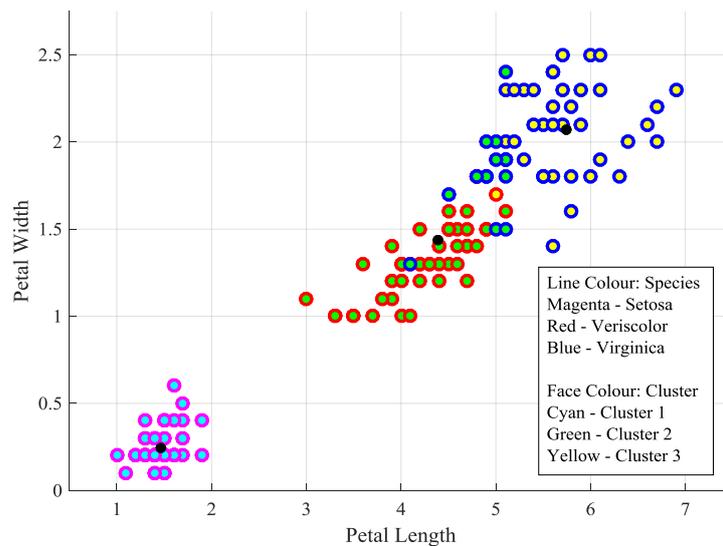
Figure 8: Iris data clustered using k-means

3.4. Summary

In this chapter, two SA techniques appropriate for exploring the behaviour of simulated complex systems have been described in detail. The first is a screening method, known as the Morris method, which is able to quickly rank the most important factors within an analysis at a low computational cost. The second is a variance-based method created by Sobol, which is more computationally expensive, but is able to quantify the difference in the importance of factors. The choice of method depends on both the number of factors and the time taken for model evaluations. When there are a large number of factors or high computational cost, Morris is preferred. Once the SA results have been generated, they must be analysed in order to gain an understanding of the system behaviour. When systems of subsystems are considered, this involves understanding not only the importance and relationships between factors in a subsystem, but the trends between subsystems also. As the data is multivariate, conventional graphical representation techniques offer a limited understanding. More sophisticated representation methods are therefore introduced, including heat and height maps, parallel coordinates, dimension stacks and star glyphs. Two pertinent techniques are also introduced which are able to analyse the trends in multivariate data: PCA and clustering. In the next chapter, a method is developed for finding solutions for complex systems which uses appropriate SA, data representation and MA techniques from those discussed in this chapter.

Chapter Four

Developing the Method

"What is necessary is the thorough knowledge of some small group of facts, the recognition of their relationship to each other, and of the formulae or laws which express scientifically their sequences"

K. Pearson (1900, pp.11-12)

4.1. Introduction

This chapter addresses research objective three, by summarising the objectives, scope and stages of the method developed in this work. Within the method description, the four research questions (d-g) associated with the objective are answered:

d. How are subsystems of systems defined?

e. How is solution suitability determined?

f. Which data should be captured in the method?

g. How is data kept consistent between subsystems?

4.2. Method Overview

Given the broad definitions of complex systems, the range of problems which can be considered to involve these and the highly specific nature of both the system and problem, it is perhaps impossible to create a one-size-fits-all approach to find solutions for complex systems; it would be arrogant to suggest that I have done so. The method that is described in this thesis is therefore aimed at addressing only one type of problem for a certain type of complex system, which I have termed a 'complex optimisation problem'.

4.2.1 Objectives

The problem is this: 'Which solutions should be implemented where?'

The solver may be trying to improve a certain aspect of a complex system and knows that a range of solutions exist, but there is a limited understanding about which of these are most

appropriate for the individual subsystems of the system; how they interact; and how they affect the overall system behaviour, making the selection something akin to guesswork. Rather than conducting a range of ad-hoc experiments, the suggested method provides a formalised experimental process so that the solver can learn comparable information about each subsystem individually, use this to gain an understanding of the relationships between subsystems, and ultimately determine 'which solutions should be implemented where'. This method works on the premise - introduced in Literature Review Section 3.1 - that systems can be optimised by optimisation of subsystems, provided the subsystem interfaces are properly defined (Wymore, 1997; Kasser 2015).

The key objectives of the method are:

1. **To determine which solutions are most suitable for each subsystem of a system**
   Depending on the ranking and relationships between solutions, this may comprise a single solution or a number of solutions. It is assumed that once found the solutions will be tailored to the system using traditional optimisation techniques, as discussed in 2.3.2.

2. **To gain an understanding of the relationships between subsystems**

   By comparing the suitable solutions for each subsystem, the solver can learn about the similarities and differences between these subsystems. This information can be used to inform future tests and system exploration, ultimately leading to greater understanding of the system behaviour.

4.2.2 Scope

Given the problem and objectives, it is clear that this method is only suitable for systems which meet the following criteria:

1. It is a system of subsystems

In order to understand the relationship between subsystems, they must exist. Although the assessment of subsystems could be applied to a single system, the benefit of the method is the ability to represent and analyse the relationships between subsystems. This is done by ensuring that the subsystem results are comparable whilst designing the experiments.

2. It can be modelled using computer simulation

In order for the suitability of solutions to be assessed, the solver must be able to, in some sense, implement them and observe the result. This is obviously not practical for a real world system due to cost, safety, organisation and a multitude of other reasons. It is crucial therefore that the system can be modelled using a computer simulation, which allows inputs to be changed and outputs observed.

3. It has numerical inputs and outputs

These inputs and outputs should be quantitative rather than qualitative to allow the relative suitability of solutions to be assessed. Quantitative data is easier to represent and compare than qualitative data, and a greater number of statistical techniques exist to analyse it.

4. A range of solutions already exist

This is a very similar point to the first. In order to assess the comparative suitability of solutions, these solutions must already be established. Depending on the investigation the solver is conducting, these solutions may or may not have already been deemed viable for the complex system under test. Often solutions in one sector can be transferred to another – assessing whether this is feasible might be part of the problem formulation.

4.3. The Method

The method explained in this section is an extended version of the method applied in Douglas et al. (2016a, 2016b)

The method centres on SA, which is used to evaluate the importance of factors for each of the system subsystems, in relation to one, or a number, of Key Performance Indicators (KPIs). The KPIs are the aspects of the system that the solver is trying to improve. The factors are chosen to relate directly to system solutions, meaning that the SA results indicate which afford the greatest subsystem improvements. The sensitivity measures for each subsystem can therefore be considered as the key outputs. However, a large amount of other data is also generated in the SA process, and this is utilised to learn more about the relationships within and between the subsystems.

Broadly speaking the method comprises 8 stages:

1. Set the scope of the system, problem and solutions to be examined

This stage requires the solver to think about the system, problem and solutions, in order to limit and define the scope of the study. It comprises activities 1-3 and 5-6 of the problem formulation process (Kasser, 2015), as described in 2.3.1, which instructs the solver to think about:

  a) the problem in terms of 'who', 'what', 'where', 'when', 'why' and 'how', to gain multiple perspectives;

  b) the stakeholders, the system behaviours and the nature of the problem;

  c) the solutions available and their feasibility in terms of operation, structure, risk and time frame;

  d) where these solutions apply in relation to the SOI and any adjacent systems;

  e) the parts of the problem which are not pertinent and can be abstracted out.

2. Determine the factors which define subsystems and partition the system

This stage builds upon activities 4, 7 and 8 of Kasser's process. The principle of hierarchies (system of subsystems) is inherent in the method. Subsystems should be partitioned based upon quantifiable factors, in such a way that there is no overlap between them, in order for solutions to be examined for each subsystem separately. For complex systems which have a number of extremely similar subsystems, e.g., planes in an airport, it is of greater interest to the solver to compare groups of similar objects rather than each individual object, e.g., long-distance vs. short range aircraft. In this case, quantifying factors and specifying the ranges these factors take for different classifications provides an easy way to categorise new objects.

3. Identify the SA factors and KPIs for the solutions within scope

Out of the factors identified, the solver needs to decide which will form part of the analysis and which will remain fixed. The factors being varied should each relate to a single solution from the set identified in stage 1, so that their sensitivity measures also relate to only one

solution. The main KPI is going to be the system aspect that the solutions aim to improve. However, this aspect may be built up from a number of outputs, which the solver wants to investigate individually. For example, the journey time for a driver may include driving time, time stuck at traffic lights, time taken to park etc. Considering these partitions offers greater insight into the system behaviours that the solutions affect. Similarly, there may be other aspects that the solver would like to improve that are secondary to the main aspect (remember, complex problems feature polytely). In the case of the car, this could be fuel consumption or carbon emissions, as well as time.

4. Develop and validate the simulation model

The model should be able to deal with changes in the input factors identified in the previous stage. If it is unable to do so, then it should be modified or a new model created. Validation ensures that the model reflects the behaviour of the real system, so that the results can be used with confidence to inform real world applications.

5. Perform SA using the factors identified, for each subsystem

The sensitivity measures, μ^* and TSI_i, generated by Morris and Sobol respectively, are comparable (Campolongo et al., 2007), meaning that the choice of SA really comes down to computational cost. For a complex system which the solver has split into subsystems defined by factor ranges, the subsystem analysis may be done on a number of test cases covering the range. This increases the computational cost, but allows the solver to learn more about the subsystem behaviour. Depending on the results, the solver may choose to do an analysis using this subsystem as the SOI. Knowledge acquisition and application are cyclical stages where the results of one experiment may reveal more areas for experimentation.

6. Analyse the relationships within subsystems

As well as ranking importance, the SA provides information regarding interactions between factors. In Morris the interaction effect is given by σ, whereas in Sobol it can be calculated by subtracting the main order effect, S_i, from the TSI_i. The visualisation and MA techniques introduced in Chapter 3 can be applied to gain an understanding of trends within the subsystem, although the selection of technique depends on the dimensionality and structure of

the data. To grasp the impact of different combinations of factors on each KPI, the input and output values for every simulation run should be retained for analysis.

7.   Analyse the relationships between subsystems

The data representation and MA techniques, introduced in Chapter 3, can also be used to analyse the relationship between subsystems. Again, the selection depends on the structure of the data, but it is likely that the individuals will be the subsystems and the variables the sensitivity measures for each factor. In order for this stage to be conducted, the SA results for each subsystem must be comparable. To ensure that this is the case:

- The SA should vary factors over a specified percentage range from a base case, where the percentage is the same for each subsystem

- The sensitivity measures should be calculated for each KPI based on their percentage difference from the result of the base case simulation conducted for each subsystem

8.   Use the results to inform in-depth simulations of solutions

Once the most suitable solutions have been found for each subsystem, in-depth simulations should be done to find the optimal solution, or combination of solutions, for the subsystem. This is normally done using an algorithm which searches for the optimal combination of factors to maximise or minimise a specified objective function.

The 8 stages of the method are summarised in Figure 9 overleaf.
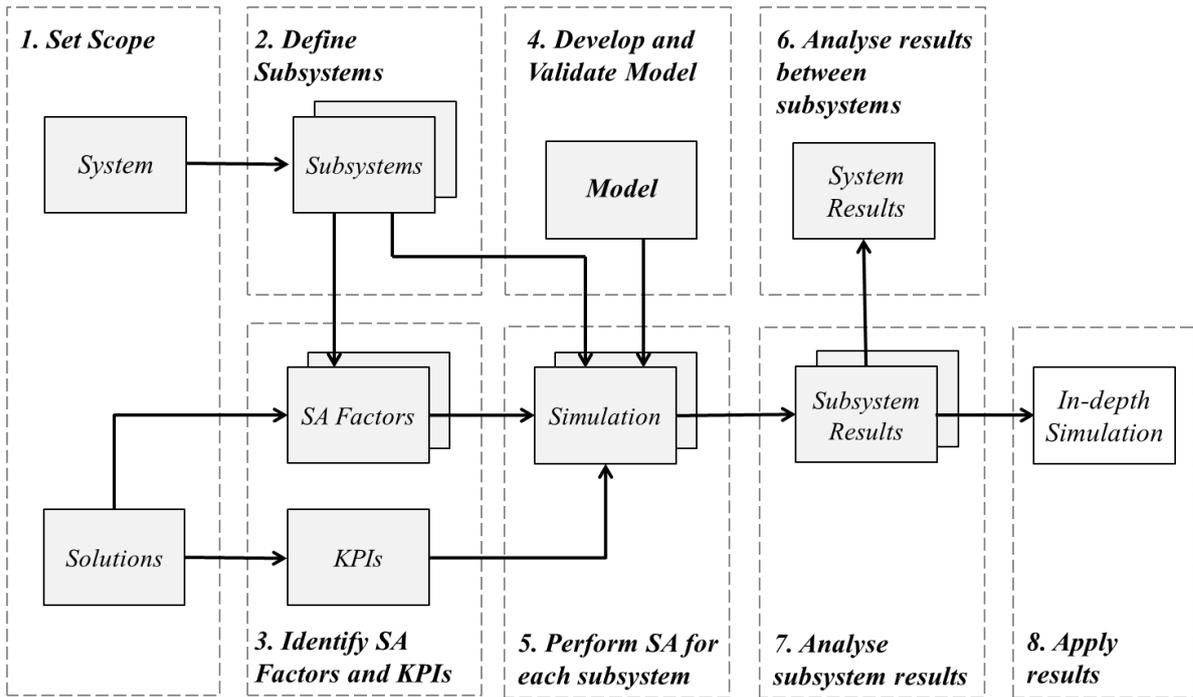
4.4. Summary

This chapter has introduced the objectives, scope and stages of the method developed in this study. The method targets complex problems focused on improving some aspect of a complex system, which comprises a number of subsystems. The method aims to determine the most suitable solutions for each subsystem from an appropriate solution set and to gain an understanding of the relationships that exist between subsystems. Research questions d-g have been addressed in the description of the method stages. To review:

d. The system subsystems are defined using quantifiable factors, in such a way that there is no overlap between them. If there are many similar subsystems, these can be grouped together by specifying these factors as taking values over a range;

e. Solution suitability is determined by choosing one appropriate SA factor to represent each solution. Therefore, when the sensitivity measures are calculated, the ranking of these factors then also indicates the ranking of solutions;

f. The data captured in the method should not only include the sensitivity measures for each subsystem, but the values of the inputs and outputs for each simulation run. This allows in-depth analysis using data visualisation and MA techniques;

g. Data is kept consistent between subsystems by specifying a base value for factors for each subsystem, ensuring the same percentage range is used to vary the factors between subsystems, and calculating the sensitivity measures from the KPIs as a percentage of the base case value.

In the following chapters the method is demonstrated through application to the problem of traction energy saving for passenger railways.

Chapter Five

Application to Rail Energy: Background

*"If we can use the next 20 years to apply existing technologies to reduce carbon emissions…
we could stop it [climate change] before it becomes catastrophic"*

B. Obama (2016)

5.1 Introduction

In this chapter I describe the application of method stages 1-4 to the problem of rail energy, which is briefly introduced below. This can be considered as the background to the analysis. The scope of the problem, solutions and system are set; the system is then partitioned into subsystems; the Sensitivity Analysis factors and Key Performance Indicators are determined; and, finally, the simulation model is introduced.

Please note: The black italicised content in Sections 5.2 and 5.3 has been taken from Douglas et al., 2015, in accordance with the Elsevier publishing agreement in Appendix B. The grey italicised content in Sections 2 and 3 has been taken from Douglas et al., 2016a, in accordance with the ICE publishing agreement in Appendix B.

Why Rail Energy?

Whilst climate change is becoming an ever more pressing issue and energy resources ever scarcer, the demand for transportation worldwide is increasing. To reduce emissions, there needs to be a modal shift to less carbon intensive transport modes, better performing vehicles and engines and an increase in the use of fuels with less carbon intensity than fossil fuels (Sims et al., 2014). Due to its inherent potential for efficiency, rail is an essential transport mode for the future. However, a modal shift to rail is not enough: to meet both passenger demand and challenging environmental targets, the railway must be improved in terms of energy efficiency.

5.2 Stage 1: Set the Scope

a) What is the problem?

There are a number of ways to reduce energy use in rail, which may involve changes to the infrastructure, operations or rolling stock on a particular network or line, or in more than one of these areas. *Through the development of accurate models and simulations, researchers are better able to predict the energy savings from implementation of these measures (Hull, 2009).* However, the majority of this research focusses on the implementation of a single solution on a simplified, specific type of railway or line section, under exact conditions. Stakeholders have limited information regarding the interactions between solutions and their transferability from one network to another, making the selection of solutions for a given network difficult. The results from this study can be used to ensure that only the most effective solutions are researched and implemented for each type of railway, thus increasing the amount of energy saved. The screening approach also ensures that time and resources are not wasted investigating the impact of ineffective solutions, further reducing costs and potentially reducing the time taken for solutions to be deployed.

b) What are the system behaviours?

The railway is a significantly complex system, both in terms of stakeholders and system behaviour. In Great Britain, the majority of train services are operated by train operating companies (TOCs) on infrastructure owned by the infrastructure manager, Network Rail, using rolling stock leased from rolling stock operating companies (ROSCOs). Various TOCs can operate on the same section of line. Train movements are controlled using a variety of different train control systems, which can include signalling, automatic train control and integrated train control systems, and differ across the network (Zhao, 2013). Journeys range from short distances within a city, to longer distances between nearby towns and cities, as well as long distance journeys across the country. In order to deliver these services a range of infrastructure and rolling stock is needed. Rolling stock can operate using either diesel or electric traction. *Currently, in the UK, approximately 60% of passenger services use electric traction, with the remainder being diesel powered (RSSB, 2010). However, with increasing pressure to reduce emissions and energy consumption in rail, diesel traction use is generally being limited. Under Network Rail's electrification programme only 51% of the UK network will be electrified, but this will supply 75% of services (Rail.co.uk, 2014). Because of this,*

only solutions for electrically supplied railways are considered. Both AC and DC power supplies can be used. Power is transformed from the national grid to the appropriate voltage and type to be used. The trains take power from the supply via overhead catenary wires or third rail, using pantographs or collector shoes respectively, and this supplies the electric equipment on board, being transformed again if needed. A number of substations are required along a route to ensure adequate power provision.

c) What are the feasible solutions?

The most feasible solutions are those that target traction energy, which in Britain can account for up to 80% of energy consumption within the railway (RSSB, 2010; Gonzáles-Gil et al., 2014). The total traction energy is defined as the energy taken from the supply less the energy regenerated to the supply. *Figure 10 shows the flow of traction energy through a vehicle. The given percentages are illustrative, and will vary depending on vehicle, route and environmental conditions. In electric traction there are conversion losses at the coupling point to the grid and further losses between the coupling point and the catenary (Hoffrichter, 2013).*
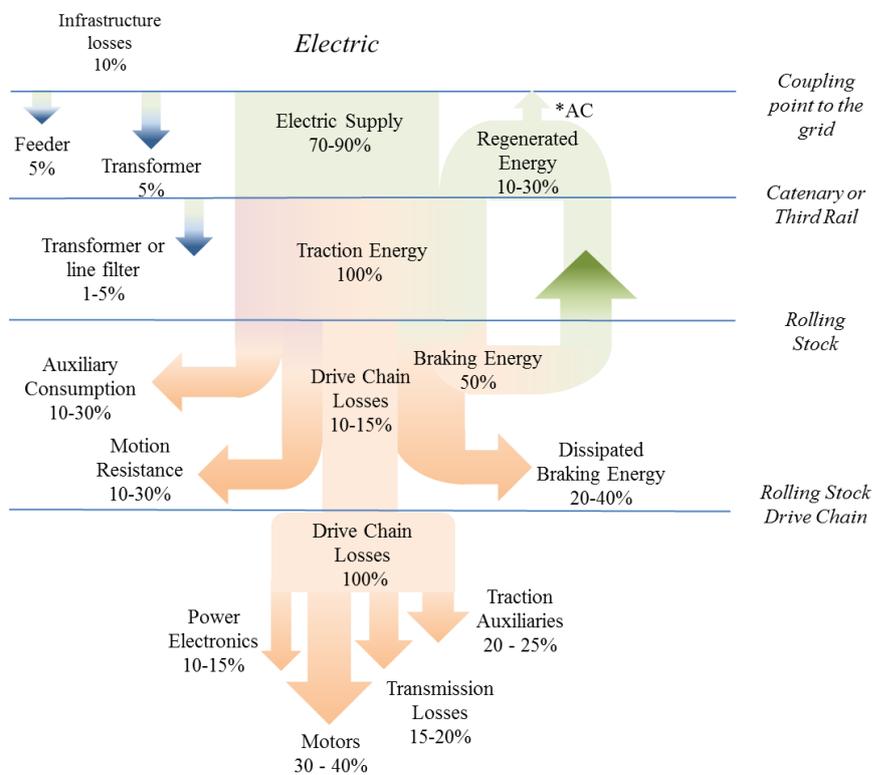
Figure 10: Traction energy flow for electrically powered vehicles (adapted from Douglas et al., 2015)

The resultant traction energy is used to propel the vehicle and power auxiliary functions, which include heating, ventilation, air conditioning (HVAC) and lighting to maintain the comfort of passengers. Overcoming the resistance to motion consumes further energy, accounting for between 10% and 30% of overall energy consumption. Motion resistance and braking can be considered together as the driving energy consumption, which will vary depending on the driving style, service speed and frequency of station stops. Typically, up to 50% of the traction energy is dissipated in braking processes. However, electric traction facilitates regeneration which significantly reduces this wastage by feeding energy back into the catenary supply for use by trains in the same section. Note that for AC railway networks, some of this energy can also be fed directly back to the grid. Drive chain losses then account for the remaining energy use. Using this understanding of energy flow, solutions can be grouped into five categories based on the energy use they target (Figure 11).
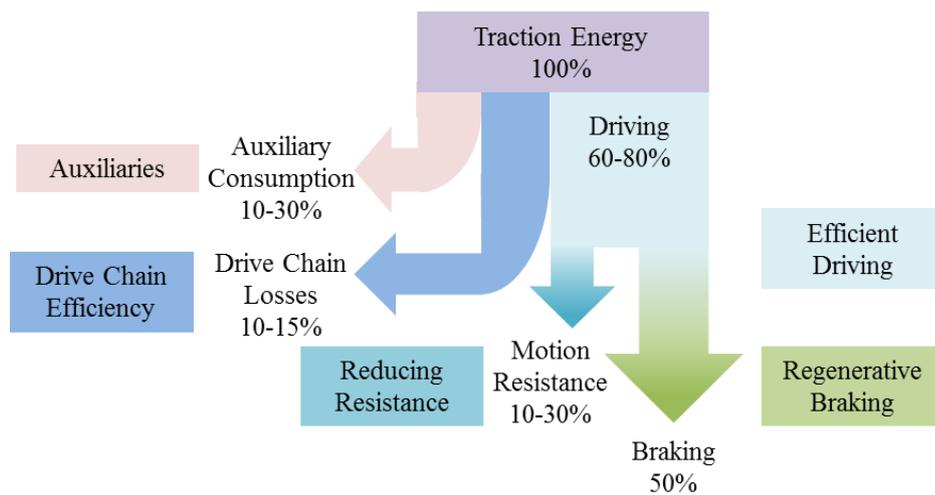
Figure 11: Solution groups based on traction energy flow (Douglas et al., 2015)

Auxiliaries

Efficient HVAC and lighting installations are one way to minimise auxiliary consumption. Savings can also be achieved through better control of existing heating and lighting equipment: by reducing temperature set points (Ticket to Kyoto, 2013); regulating fresh air intake (Kokken, 2003); or reducing light levels (RSSB, 2007). *Thermal insulation is another key area which can reduce consumption, by minimising heat transfer in and out of vehicles (RSSB, 2007). This involves choosing appropriate materials to thermally insulate walls, doors, windows, floors and ceilings.*

Drive Chain Efficiency

The major source of loss within the drive chain is motor inefficiency (Kondo et al., 2014). Current AC motors can be redesigned to improve efficiency by using higher-grade core materials, using higher conductivity rotor bars, reducing harmonics or optimising the stator winding design (Kondo et al., 2014; 2008, Matsuoka and Kondo, 2010). An alternative high-efficiency motor technology is the Permanent Magnet Synchronous Motor (PMSM), which is currently being used in Japan (Sato et al., 2010) and France (Soulard, 2012). PMSMs can achieve efficiencies of up to 97%, by using permanent magnets to generate a field, rather than relying on the field produced by the rotor currents, thus reducing losses (Gieras and Wing, 2002).

Reducing Resistance

Solutions to minimise this consumption become apparent when considering the equation of train motion, as described by Lomonosoff (1933). Acceleration, a, is calculated by taking the resistive forces, W, from the propulsion force, F_S, and dividing by the inertial mass, M_E. The inertial mass includes a constant, λ, allowing for rotating parts and is calculated as $M(1 + \lambda)$.

$$a = \frac{F_S - W}{M_E}$$

To achieve the same acceleration using less propulsive force, and therefore less energy, either the train mass or resistive forces, or both, must be reduced. Mass can be reduced by introducing lightweight materials, components and construction techniques during design or retrofit (Gonzales-Gil et al., 2014), focussing particularly on the equipment, propulsion, interior and car body structure (Koenig, 2011). W comprises resistance to motion and resistance from gradient. As gradient change would require significant modification of route layout and infrastructure, it is not considered a viable option for existing railways. The resistance to motion, F_R, is generally described by the Davis equation, $F_R = cv^2 + bv + a$ (Rochard and Schmid, 2000). a and b are mass-related coefficients, whereas c depends on aerodynamic design. The c coefficient, and therefore the overall resistive force, *can be reduced by improving the aerodynamics of the vehicle, through optimisation of the front and back ends, spoilers, pantograph integration and bogie space envelope (Bombardier*

Transportation, 2010). Another option is to reduce the maximum operating speed where possible. This is of particular significance on high speed lines, which consume a large amount of energy overcoming resistance (Hasegawa et al., 2014).

Regenerative Braking

Rail vehicles with electric motors can use them to brake electrically, recovering up to a third of traction energy in the process. In this mode - commonly known as dynamic or regenerative braking - the motor torque opposes rotation slowing the vehicle and generating power. This regenerated energy is normally more than sufficient to supply on-board auxiliaries, leaving excess (Gonzales-Gil et al., 2014). In electrified networks this excess can be returned to the supply to power other trains in the same section. In AC networks, the excess feeds directly back into the grid. *However, if the network is unreceptive, i.e., there is nothing to use the energy, or if it is non-electrified, the energy is wasted as heat in resistors. A recent review of literature (Gonzales-Gil et al., 2013) shows that the main regenerative energy saving measures are: optimising operating timetables to maximise energy exchange between vehicles, implementing reversible substations to supply regenerated energy to the national power grid and using on-board Energy Storage Systems (ESS) or Wayside Energy Storage Systems (WESS) to capture and reuse braking energy when needed. Several studies also focus on ensuring effective regeneration to maximise energy recovery by modifying vehicle braking systems or trajectories (Lu et al., 2014; Wang et al., 2010).*

Efficient Driving

Drivers can primarily save energy on a journey by introducing one or more 'coasting' phases, where power is not applied and the train decelerates because of resistive forces. This can be easily implemented by educating drivers about eco-driving techniques (RSSB, 2011) or installing coasting boards at trackside which indicate when to coast (Coleman et al., 2010). The trade-off between the energy saved and increased journey time must be managed. For a given route, an optimum trajectory can be calculated which combines acceleration, speed-holding, coasting and braking phases to minimise energy consumption whilst meeting timetable requirements. In such a trajectory, not only coasting can be optimised but the holding speeds, and acceleration and braking curves. To implement these trajectories Driver Advisory Systems (DAS) can be installed in-cab to: generate energy efficient trajectories, give instructions to drivers, monitor the train movement and update trajectories as needed (Panou

et al., 2013). However, the success of these systems relies on the drivers understanding and trusting the instructions given. Automatic Train Operation (ATO) negates the need for a driver, meaning energy efficient trajectories can be implemented more easily. *However, there are technical difficulties in safely and efficiently controlling a running train due to disturbance, noise in measurements and the non-linearity of train motion dynamics (Li et al., 2013).*

Figure 12 summarises the solutions available within each group. Each solution can be classified as either a procedure or technology which can be applied to the infrastructure, rolling stock or service of a railway. Technologies are physical changes, systems or equipment to be incorporated into the railway system. Procedures are alternative ways to reduce energy, either through design or processes. Control strategies which may rely on new control technology are categorised as procedures due to a relatively low implementation cost.

Figure 12: Main solutions available to reduce traction energy use (adapted from Douglas et al., 2015)

The potential savings and implementation costs of each solution are given in Table 6. These numbers have been taken from Table 6 in Douglas et al., 2015, which used 79 sources to derive the approximate saving percentages. It is important to note that the percentage savings represent the maximum potential saving of a solution implemented in isolation and that some

of these percentages are additive and others are not. In some instances there can be positive interactions between solutions. Upgraded equipment, for example, is often lighter than its predecessor, which reduces vehicle mass and leads to further savings. However, implementation of one solution may also limit the effectiveness of another solution. On a railway which uses timetable optimisation to ensure the exchange of braking energy between vehicles, energy storage systems may be redundant. Interactions are discussed further in Douglas et al., 2015.

The percentage savings in Table 6 give a good indication of the feasible solutions (high saving, low cost). However, all high and medium saving solutions are considered viable within this study. A number of high cost solutions (aerodynamic design, permanent magnet motors, automatic train operation) would be implemented during the design stage of a vehicle, thus representing a one-off cost to be returned over the lifetime of the rolling stock. Equally, the cost of implementation does not give an indication of the secondary benefits solutions can offer, such as reduced maintenance costs for train and track, longer lifecycle, improved performance, improved passenger comfort, greater network capacity or greater appeal for passengers.

Table 6: Potential savings of traction energy solutions (adapted from Douglas et al., 2015)

Solutions		Maximum Potential Saving, %	Cost
Auxiliaries	HVAC and Lighting	7	Low
	Thermal Insulation	5	Med
Drive Chain Efficiency	Motor Power Control	7	Low
	Drive Chain Control	3	Low
	Permanent Magnet Motors	20	High
Reducing Resistance	Mass	15	Med
	Aerodynamic Design	15	High
	Maximum Speed Limit	25	Low
Regenerative Braking	Wayside Energy Storage	35	High
	Reversible Substations	20	High
	On board Energy Storage	35	High
	Timetable Optimisation	15	Low
Efficient Driving	Eco driving	35	Low
	Traffic Management	15	High
	Driver Advisory Systems	20	Med
	Automatic Train Operation	30	High

* Traffic light for maximum potential saving defined as follows: red <10%, >10% orange <20%, green >20%

d) Where are these solutions applied?

Considering only high and medium saving solutions, Table 7 summarises where the solutions apply in terms of infrastructure, rolling stock and service.

Table 7: The application areas of traction energy solutions

Solutions		Solution Application
Drive Chain Efficiency	Permanent Magnet Motors	Rolling Stock
Reducing Resistance	Mass	Rolling Stock
	Aerodynamic Design	Rolling Stock
	Maximum Speed Limit	Service
Regenerative Braking	Wayside Energy Storage	Infrastructure
	Reversible Substations	Infrastructure
	On board Energy Storage	Rolling Stock
	Timetable Optimisation	Service
Efficient Driving	Eco driving	Service
	Traffic Management	Service
	Driver Advisory Systems	Rolling Stock
	Automatic Train Operation	Rolling Stock

Summary of Scope

The problem is concerned with finding the most appropriate solutions to save **traction energy** for different types of **electrified railway**. Feasible solutions are split into four categories: improving the drive chain efficiency, reducing motion resistance, maximising regenerative braking use and efficient driving.

5.3 Stage 2: Partition the System

Different railways can generally be categorised based on the network on which they operate, and the service which they deliver. In order to meet the service requirements different rolling stock are required for each network type and service. Loosely speaking, railway networks can be categorised as one of three types: Urban, Inter-city or High Speed (HS), and services as Urban, Commuter and High Speed. Each network is powered using either AC or DC electrification, as summarised in Table 8 (Schmid and Goodman, 2014). *25kV AC is defined as the target supply for all new lines, including HS, in the Technical Specification for Interoperability (RSSB, 2012).*

Table 8: Typical power supplies for each network type

Type	Voltage	Urban	Inter-city	High Speed
DC	400-1200	■		
	1500	■	■	
	3,000		■	
AC	25,000		■	■

5.3.1 Network Descriptions

5.3.1.1 Urban Network

Urban rail transport generally refers to railway systems in metropolitan areas which provide public transport (Gonzales-Gil et al., 2014). Tramways excluded, they can be defined as having three modes: light rail, rapid rail and regional or commuter rail transport (Vuchic, 2007). Typically light and rapid rail systems are operated on a fully separated, electrified right of way, whereas regional or commuter rail is operated utilising electric or diesel traction on lines with mixed traffic, which can include freight and intercity services. As the line is categorised separately from the service in this evaluation, 'urban' is only applicable to fully separated electrified lines, such as metros.

Urban networks aim to transport a high volume of passengers quickly and easily around all areas of a city. This leads to a number of distinguishing features: short headway and dwell time, a high number of stations with short interstation distances, and a low commercial average speed. Services normally stop at every station along the route, as limited space typically means a single track line in each direction with no overtaking facilities. Running a high frequency, high capacity service, achieved by using a single stock type, allows passengers to take the next available train rather than a timetabled service. There are typically few seats with the majority of passengers standing. At 'crush' loading there can be over three times the amount of passengers standing to sitting, assuming 7 passengers per m^2 of floor space (London Underground, 2011).

5.3.1.2 High Speed Network

High Speed Rail (HS) is similar to Urban Rail in the sense that traffic tends to operate on a fully separated, electrified right of way. In some cases, as with the UK line High Speed One (HS1), high speed freight traffic may take advantage of the route to deliver time critical commodities (HS1, 2015). However, passenger traffic tends to be of the same type to ensure a

reliable high speed service. The European Union defines HS as having two components: infrastructure specially built or upgraded for high speed travel above 200 km/h; and advanced technology trains designed to guarantee safe, uninterrupted travel at such speeds. The compatibility between these components is also assumed to be excellent in order to achieve the required level of service (European Commission, 1996). The International Union of Railways, recognises that 'high speed traffic' running at significant speeds on conventional lines might be categorised as HS in countries with a low performing conventional railway (UIC, 2017). However, higher speed services running on conventional, mixed traffic lines are categorised separately in this work.

High speed networks aim to transport large numbers of passengers quickly between important destinations domestically or internationally. As well as the distinguishing high operational speed, characteristics conducive to this aim include: long interstation distances with few stations stops along a route; large capacity and train length; and all passengers seated for both comfort and safety.

5.3.1.3 Inter-city Network

This definition encompasses anything not directly covered by the previously outlined Urban and High Speed Rail networks. Inter-city comprises mixed traffic lines, running a wide variety of passenger services and freight. The speed limit may be high, but still considerably lower than that of High Speed rail. Different services require different rolling stock capabilities, which can limit the overall line capacity due to differing braking distances. However, lines often have multiple tracks in parallel to alleviate this problem. For example the East Coast Main Line in the UK has, for the most part, quadruple track from London King's Cross to Stevenage (Network Rail, 2010). The line can be of significant length and have a high number of stations, but not every service will stop at all stations along the route. There also tends to be a smaller number of passenger journeys per km of rail, than both Urban and High Speed, on lines of this type.

5.3.2 Service Descriptions

5.3.2.1 Urban Service

Urban services are specific to segregated urban lines and aim to satisfy inner-city public transportation needs. They are extremely high frequency services: some running in excess of

30 trains per hour (Transport for London, 2014). Dwell times are minimised to maximise service frequency. As such, the carriages are designed for the majority of passengers to stand, which reduces the time to alight and disembark at stations, whilst also increasing the maximum vehicle capacity. The interstation distance is short, allowing passengers to travel short distances across the city.

5.3.2.2 Commuter Service

Commuter services are designed for work trips and may only operate during peak hours (Vuchic, 2007). There is typically less demand for commuter rail than urban rail so consist-length, frequency and capacity are lower. The interstation distance is longer than that of urban services, although not always by a considerable amount. Commuter rail services exist on both Inter-city and High Speed networks, with those on HS travelling faster and greater distances. Some metro services which connect outlying parts of the city can also be categorised as Commuter rail in terms of service frequency and capacity.

5.3.2.3 High Speed Service

High speed services are distinguishable by high speed and high capacity. Interstation distance is long, with few stations along a route. The service frequency is lower than that of Commuter services, and dwell time is longer to allow passengers to alight at stations. High Speed services on mixed lines generally operate at a lower speed than services on dedicated HS infrastructure, with lower capacity and longer dwell time.

5.3.3 Quantifying Networks and Services

Based on the descriptions in the previous section, a range of characteristics have been selected to describe both networks and services (Tables 9 and 10). *Each characteristic has been assigned four ranges of values, with 1 representing a low value and 4 a high value for the given characteristic.* The only qualitative descriptions are those of service patterns and mix of rolling stock, which relate to one another. For service patterns a number 1 represents a network which only runs a single service whereas a 4 represents a network where the services are extremely diverse e.g. both local stopping services and long distance high speed services use the same line. For mix of rolling stock, a 1 represents complete homogeneity of stock whereas a 4 correlates to the range of rolling stock needed to run the varied service patterns

described above. A service on a given section of line can easily be assigned a network and service type based on this quantification.

Table 9: Network characteristics and value ranges (Douglas et al., 2015)

	Characteristic	1	2	3	4
1	Line Speed Limit, v: km/h	$v <= 80$	$80 < v <= 160$	$160 < v < 250$	$v >= 250$
2	Number of parallel tracks	1	2	3	4
3	Line length, x: km	$x <= 20$	$20 < x < 100$	$100 <= x < 250$	$x >= 250$
4	Number of stations	1-5	6-20	21-50	51+
5	Number of operators	1	2	3-5	6+
6	Number of passenger journeys, j: thousands per km of line	$j < 100$	$100 <= j < 200$	$200 <= j < 500$	$j >= 250$
7	Service patterns	Single	Small variances	Many variances	Extremely varied
8	Mix of rolling stock	Single	Similar	Mixed	Very Mixed
9	Number of stock types	1	2-4	5-8	9+

Table 10: Service characteristics and value ranges (Douglas et al., 2016a)

	Characteristic	1	2	3	4
1	Trains per hour, tph	1-2	3-6	7-15	15+
2	Number of cars	1-4	5-8	9-12	13+
3	Capacity, n	<250	$250 <= n < 500$	$500 <= n < 750$	$n >= 750$
4	Ratio of Seated to Standing Passengers, n_r: %	<25	$25 <= n_r < 50$	$50 <= n_r < 75$	$n_r >= 75$
5	Interstation distance, x_i: km	$<= 3$	$3 < x_i <= 20$	$20 < x_i < 50$	$x_i >= 50$
6	Dwell time, t: min	$<= 1$	$1 < t <= 2$	$2 < t < 5$	$t >= 5$
7	Maximum Speed, v: km/h	$v <= 80$	$80 < v <= 160$	$160 < v < 250$	$v >= 250$

5.3.4 Subsystems

The subsystems for the analysis can be created using the definition and quantification of networks and services. Commonly, these would be referred to as sub-modes of the system railway. However, I have chosen to adopt the term subsystems in order to be aligned with the definitions in the methodology. The characteristic values for each network type are shown in Figure 13. Given that only certain services are able to operate on certain networks, there are only 6 subsystems (Table 11). The typical service characteristics for each of these subsystems are shown in Figure 14. *To meet their operational requirements, the vehicles providing the services on each network differ. They need to achieve different maximum speeds, accelerations and capacities, which influence the design of their body, interior and drive*

chain. The drive chain design depends on the power supply infrastructure, which is either AC or DC supplied by third rail or OLE.

Table 11: Railway subsystems categorised by network and service type

Service/Network	Urban	Inter-city	High Speed
Urban			
Commuter			
High Speed			
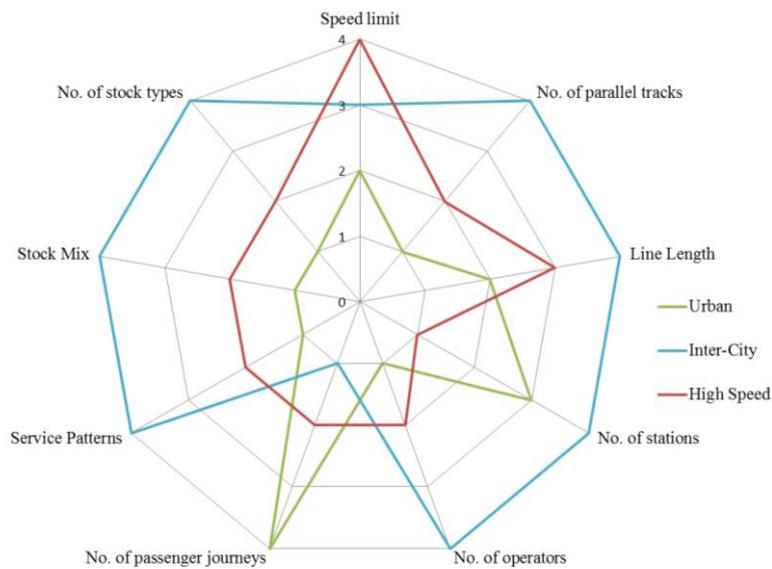
Figure 13: Typical characteristic values for each type of network (Douglas et al., 2015)
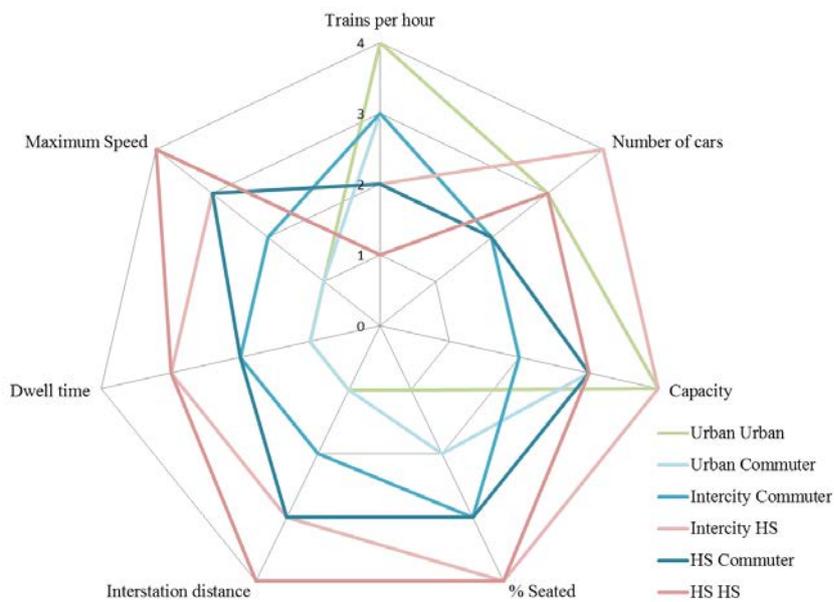
Figure 14: Typical characteristic values for each railway subsystem

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Examples from Great Britain for each of the subsystems are (service, network):

- Urban, Urban: S-Stock, operating on London Underground

- Commuter, Urban: Class 378, operating on London Overground

- Commuter, Inter-city: Class 350 Desiro, operating on the West Coast Main Line

- High Speed, Inter-city: Class 390 Pendolino, operating on the West Coast Main Line

- Commuter, High Speed: Class 395 Javelin, operating on High Speed One

- High Speed, High Speed: Class 373 Eurostar, operating on High Speed One

5.4 Stage 3: SA Factors and KPIs

Each of the factors chosen for sensitivity analysis should relate to a single solution in order for the importance ranking to be attributed to that solution. This is straightforward for the solutions to reduce motion resistance and improve drive chain efficiency. However, both regenerative braking and efficient driving solutions require more thought. The optimal solution to increase regenerative braking greatly depends on not just the network and service, but the power supply, infrastructure, existing timetable and overall behaviour of the specific case (study) within the subsystem. Trying to incorporate this level of complexity in a screening method would be detrimental to the analysis, increasing both the number of simulation runs and the model computation time. It would be better to consider the importance of regenerative braking overall and then, if it is a pertinent factor, to conduct experiments to determine the most suitable solution from this group. The same can be said of efficient driving solutions. The suitability of DAS, ATO and traffic management systems depends on the individual routes of each case study, the ease of implementation and susceptibility to delay. Instead of including all of these variables, the impact of incorporating coasting phases can be evaluated. This is a key feature of trajectory optimisation and therefore indicates whether efficient driving techniques (however they are implemented) are suitable for the subsystem. The SA factors which relate to each solution are detailed in Table 12.

Table 12: The SA factors relating to each of the solutions identified in Chapter 5 Section 3

Solution Group	Solution	SA Factor
Drive Chain Efficiency	Permanent Magnet Motors	Motor Efficiency
Reducing Resistance	Mass	Mass
	Aerodynamic Design	Aerodynamics
	Maximum Speed Limit	Maximum Speed
Regenerative Braking	Wayside Energy Storage	Regenerative Braking Use
	Reversible Substations	
	On board Energy Storage	
	Timetable Optimisation	
Efficient Driving	Eco driving	Coasting Phases
	Traffic Management	
	Driver Advisory Systems	
	Automatic Train Operation	

The main KPI for this analysis is the total traction energy, which is defined as the energy taken from the supply less the energy regenerated to the supply. Another important performance indicator is journey time, as some solutions will cause the journey time to increase, which is undesirable for services focused on speed.

5.5 Stage 4: Simulation Model

The factors to be analysed all relate to a single vehicle delivering a service on a specified network route. Although a multiple train scenario would give insight into the effect of train interactions, these would only occur in the case of delay or perturbation: timetables are constructed to ensure all trains are able to travel freely. Simulating a single train simplifies the model thereby reducing the computation time, which is desirable for a screening method.

The Single Train Simulator (STS), developed by Hillmansen and Roberts (2007), was chosen to complete the analysis. The user is able to specify both route data, covering service and network variables, and vehicle data. The train movement is then calculated using Lomonosoff's equation using discrete distance steps. Based on the acceleration profile of the vehicle, the tractive effort and subsequent power and energy requirements can be derived. Losses in the drive chain are accounted for by a 'generation rate' variable. For example, if the generation rate is 0.85 this means only 85% of the power from the catenary reaches the motor, i.e., 15% is lost in the drive chain. Dividing the power requirement of the motor by the generation rate therefore gives the power drawn from the catenary. A similar variable, 'regeneration rate', accounts for the losses in regeneration back to the line. Regeneration to

the auxiliaries is negated, meaning this is the same as the generation rate (Douglas et al., 2016c). The total energy requirement of the train is the energy required from the catenary less the energy regenerated back to the line.

The STS has previously been validated against real world data, and before use in this analysis was validated using a new analytical method, which ensures the dynamics of train motion are correctly programmed. Further detail on the STS programming and validation can be found in Douglas et al. (2017) and Hillmansen and Roberts (2007).

5.6 Summary

The problem of selecting traction energy saving solutions for different railway types has been introduced in this chapter, and has been shown to be suitable for implementing the developed method. Method stages 1-4 have been applied to establish the subsystems; determine the SA factors for feasible solutions; find the KPIs; and establish the model to be used within the experimental analysis. Three network types - Urban, Inter-city and High Speed - and service types – Urban, Commuter and High Speed – have been categorised using quantified characteristics. Six subsystems are defined using these network and service types respectively: Urban Urban (UU), Urban Commuter (UComm), Inter-city Commuter (ICComm), Inter-city High Speed (ICHS), High Speed Commuter (HSComm) and High Speed High Speed (HSHS). The feasible solutions were found to be: improving the motor, reducing mass, improving aerodynamics, reducing the maximum speed limit, increasing regenerative braking use and implementing efficient driving. These relate directly to the factors: mass, aerodynamics, maximum speed, regenerative braking use, coasting phases and motor efficiency, the latter of which will be considered in detail in chapter 7 through a study of the implementation of PMSM in each subsystem. The main KPI is the traction energy consumption, with journey time as a secondary KPI. The following chapter uses this background information to implement the experimental analysis.

Chapter Six

Application to Rail Energy: Implementation

"Determine that the thing can and shall be done, and then we shall find the way"

A. Lincoln (1848, p.152)

6.1 Introduction

This chapter, building on the background, addresses research objective four, demonstrating the suitability of the screening method and data visualisation techniques through application to the problem of rail energy. This chapter specifically covers Method Stages 5-7. The implementation of the SA is described in detail, then the results for each subsystem are introduced and analysed. PCA is used, alongside other visualisation techniques, to determine the trends between factors and KPIs. Following the individual subsystem results, the relationships between subsystems are explored. This chapter by its very nature also explores the three sub-hypotheses: do the suitable solutions for railways differ depending on the network and service characteristics of the given railway; can these differences be used to determine the relationships between the different networks and services; and can the results be used to inform further experiments?

6.2 Stage 5: Implementation

The core of the implementation is the SA of the 6 factors identified in Stage 3 over typical ranges for each subsystem. However, in order to learn more about the subsystem behaviour for specific cases a number of test scenarios for each subsystem are established using two other important factors: the interstation distance and route gradient. Briefly exploring the effect of these 'external' factors will indicate whether the fixed route infrastructure, which is not easily or cheaply amended, impacts the suitability of solutions. If it does have an impact, the exploration will offer information on where the impact is greatest, indicating further test scenarios and possibly leading to model amendments. Each external factor is explored separately to ensure that trends are clearly attributable to either the interstation distance or gradient. To determine the sensitivity of importance to the external factors, the SA of the 'internal' factors must be completed over a range of external factor values. This requires a

layered analysis which significantly increases the number of simulation runs, as illustrated in Figure 15.

In order to minimize the number of simulation runs, and the subsequent computation time, the Morris SA method is chosen to conduct the analysis. Instead of using a low *r* value, which may lead to errors (Campolongo et al., 2007), an appropriate *r* value is chosen for the scale of the problem, based on the evaluation of a g-function.
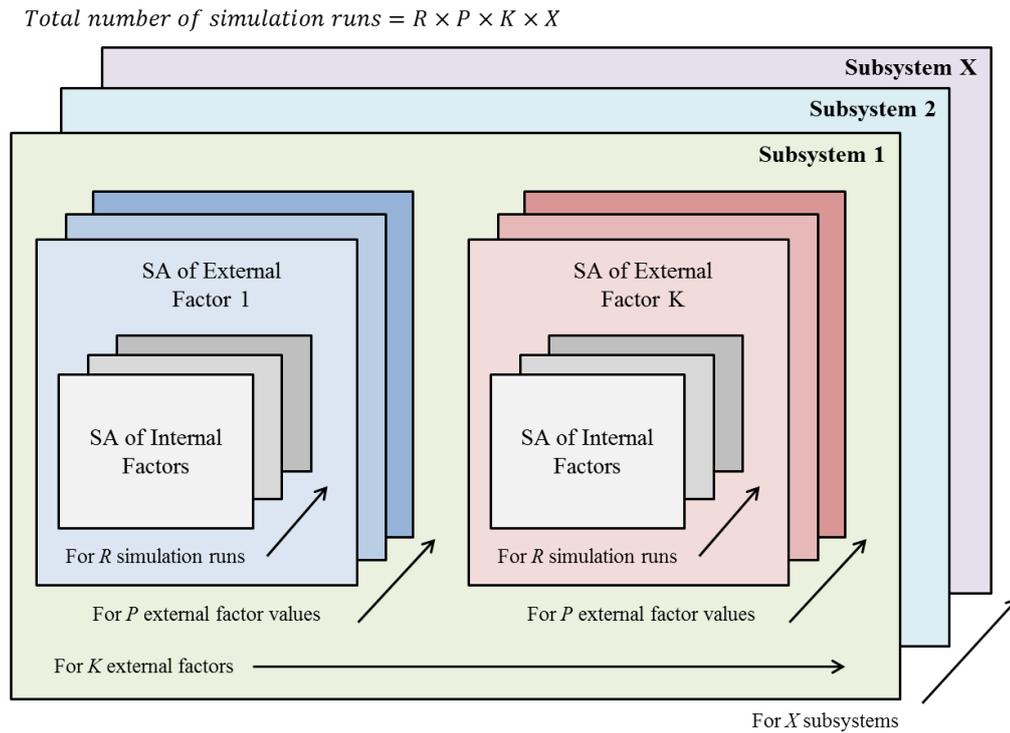
Figure 15: Scaling of simulation runs from layered analysis

6.2.1 Determining an appropriate *r* value

G-functions are non-monotonic functions commonly used as a test function for SA methods, since the solver can preset the importance of factors (Sobol, 2001; Campolongo et al., 2007; Nguyen and Reiter, 2015). The g-function used by Sobol (2001) is defined as follows:

$$g = \prod_{i=1}^{n} \frac{|4x_i - 2| + a_i}{(1 + a_i)}$$

The higher the value of a_i (which must be non-zero), the more important the corresponding factor x_i is. The hardest situation to identify would be when all of the factors are equally

important (or unimportant). In reality, all factors being equal is unlikely to occur which means that the *r* value able to identify this test case should be able to find the correct ranking for a complex model in which there are a few important factors. The above g-function is set to have 6 equally important factors, and evaluated using Morris SA with *p* =10 levels, beginning with an *r* value of 10 and incremented by 10 until the total sum of squares (TSS) is within 5% of the mean.

$$TSS = \sum_{i=1}^{n}(y_i - \bar{y})^2$$

In this case y_i is the μ^* value of factor *i,* and $\bar{y}$ is the mean of the μ^* values for all 6 factors. A high *p* value should be coupled with a high choice of *r* to ensure that all *p* levels are explored for each factor (Saltelli et al., 2004). Since a high number of trajectories are to be used (>50), *p*=10 levels is suitable to ensure exploration of all levels. Figure 16 shows the μ^* values for a test which reaches $TSS < 0.05\bar{y}$ at *r* = 450 trajectories.
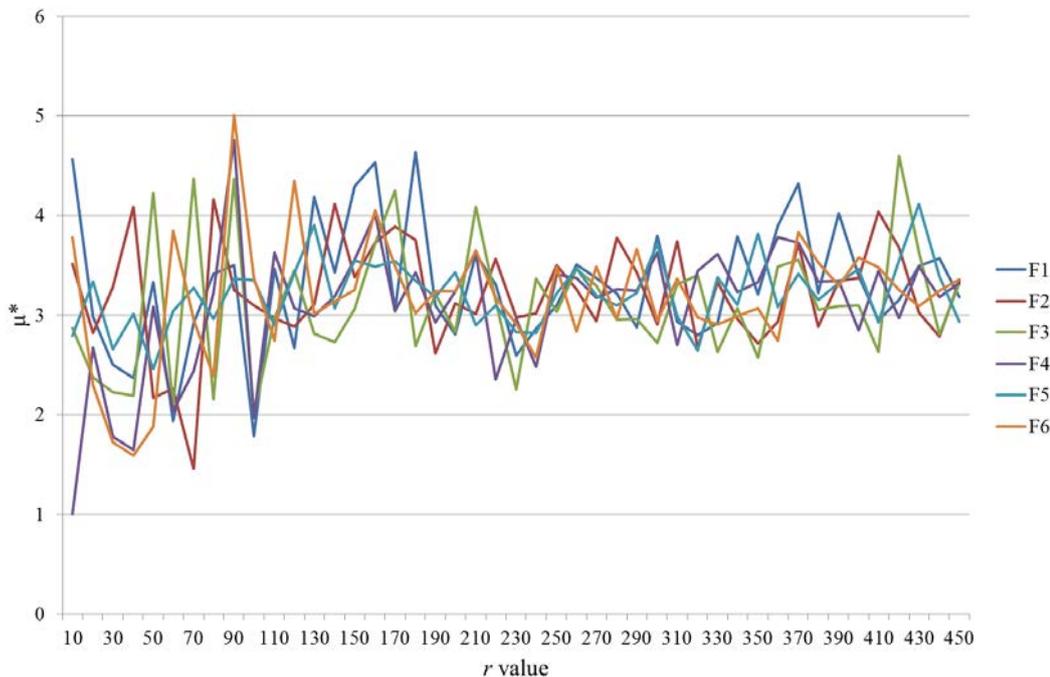
Figure 16: μ^* values for a g-function test which reaches the convergence criterion at *r* = 450 trajectories

Because the trajectories are randomly generated, some sets of trajectories may outperform others meaning that the required *r* value is less. To ensure that the correct value is chosen, the test was repeated 10,000 times. The histogram of results (Figure 17) indicates that the correct

ranking is commonly found when *r* is approximately 350, but in extreme cases almost 800 trajectories may need to be evaluated. Approximating the histogram to a normal distribution with a mean and standard deviation calculated from the 10,000 evaluations, the two sigma rule can be used to determine a suitable value for *r*. The rule states that 95% of all of the values lie within two standard deviations of the mean. The upper limit is given by:

$$r = \mu + 2\sigma = 329 + 2*114 = 557$$
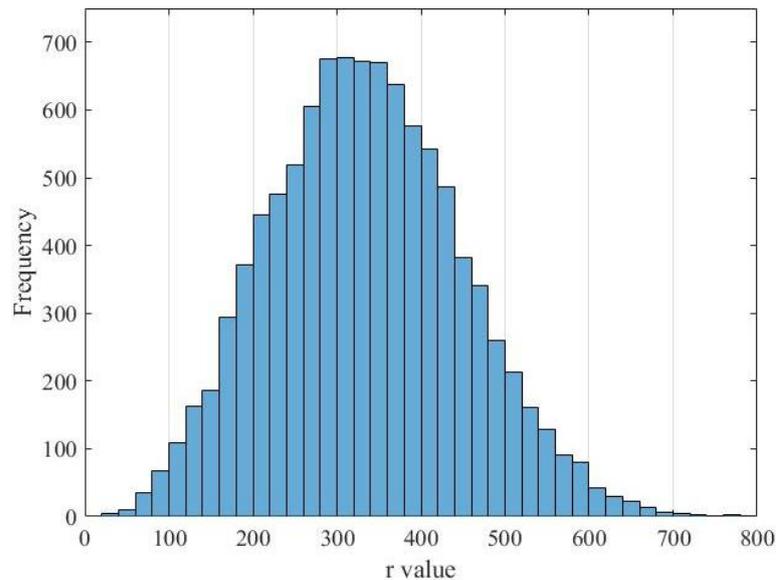
Figure 17: Histogram of minimum r values for 10,000 evaluations of the g-function test case

Based on this analysis, 560 is chosen as the *r* value for the Morris analysis of the rail energy solutions, which are to be evaluated using *p* =10 levels.

6.2.2 Simulation Procedure

To ensure that the results are comparable between case studies and subsystems, the same number of factors, levels and trajectories are used for each simulation. As described in the method section, a base value for each factor is specified for each subsystem and varied over a given percentage range, which is consistent between subsystems. For each SA evaluation, *r* trajectories are randomly generated with factor values between 0 and 1. These are then transformed to match the percentage range set for each factor (see Tables 13 and 14) and the delta value also updated. The sensitivity measures for each KPI are calculated as a percentage of the base case value, also to ensure comparability. The simulation procedure is illustrated in Figure 18.

Line length
Efficiency
Mass
Aerodynamics
Maximum
Speed
Regenerative
Braking Use
Coasting
Speed

Gradient
Interstation
Distance

Factor
ranges

Set Morris
parameters

k, p, r

For each case study

Set base case
factor values

**For each external
factor**

**For each external
factor value**

Calculate
base case
results

Generate r
trajectories

Transform
trajectories

Calculate μ,
μ* and σ

External
factor
analysis

Subsystem
analysis

System
Analysis

For each trajectory

For each step

Increase one
factor by Δ

Simulate
train run

Save KPIs

Convert to %
of base case

Calculate EE

Action

Input

Result

——— Step

——— Loop

— · — Input

Figure 18: Simulation procedure for rail energy application of the method

As well as specifying the base case values of the 6 SA factors at the beginning of the subsystem analyses, the line length for that subsystem is also specified. As the interstation distance is changed, the number of stations is recalculated using the line length. The base case results are updated after each external factor change due to the large influence these factors have on energy consumption. The same number of levels, p=10 are used for the external

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factors to extract any trends attributable to these factors. For interstation distance, these 10 levels are evenly spaced based on the minimum and maximum values specified for each subsystem (see Table 13). The gradient is also varied over 10 levels evenly spaced between ± 0.01 radians, which is equivalent to gaining or losing 10 m for every 1000 m travelled (Figure 19). The steepest gradient on Network Rail's mainline infrastructure is approximately 0.027 radians (Network Rail, n.d). The interstation distance value for the gradient analysis is the mid-point of the minimum and maximum interstation distances specified for each subsystem.
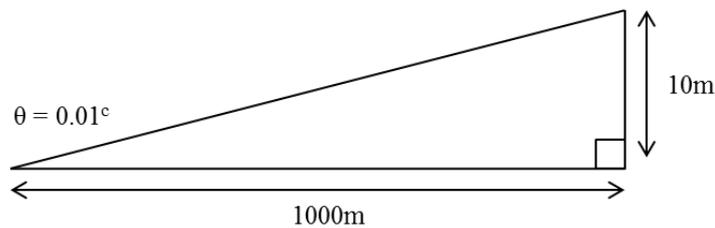
Figure 19: Illustration of the maximum gradient simulated

Updating Factor Values

This section describes in detail the simulation of each factor, and the model changes necessary when each factor is updated.

Efficiency

The motor efficiency improvements are simulated using the general efficiency variable – generation rate – which is described in Section 5.5. This is set to 0.85, simulating a 15% loss in the drive chain, which is typical for electric vehicles (see Figure 10, Section 5.1). Upgrading induction motors to PMSMs can reduce losses by approximately 7%. Based on this, a base case value of 0.85 is used and a percentage range of ±7%, which varies the efficiency from approximately 0.79 to 0.91.

Mass

The original vehicle mass is varied over ±10%, which was considered to be a feasible change in a metro light-weighting study (Carruthers et al., 2009). Changing the vehicle mass requires other simulation variables to be updated, such as the inertial mass, maximum traction and maximum acceleration. The inertial mass is calculated using the constant λ which accounts for the additional inertia due to rotating components.

$$M_E = M(1 + \lambda).$$

The maximum traction force on level ground is given by the normal force multiplied by the coefficient of friction, μ (Lu et al., 2010). On level ground, the normal force is simply the weight over the driven wheels. If only half of the axles are powered,

$$F_{Tmaz} = \frac{1}{2}Mg\mu$$

where g is the acceleration due to gravity. The maximum acceleration is recalculated using these updated variables.

$$a_{max} = \frac{F_{Tmax}}{M_E}.$$

The a and b Davis parameters, which are used to estimate the resistance to motion of the vehicle, also depend on the mass if the Armstrong and Swift calculations are used as recommended by Rochard and Schmid (2000). Normally the parameters which satisfy the Davis equation, $F_R = cv^2 + bv + a$, are determined by measurements taken during a run-down test for a given vehicle. However, such measurements do not exist for the simulated change in vehicle mass and must therefore be estimated. They are calculated as follows, where M_T is the mass of trailer cars, M_P the mass of powered cars, N_T the number of trailer cars, N_P the number of powered cars and P the total power. All masses should be in tonnes and power in kW to give a in N and b in Ns/m respectively.

$$a = 6.4M_T + 8M_P$$

$$b = 0.18M + N_T + 0.005PN_P$$

Aerodynamics

The c parameter of the Davis equation largely accounts for the aerodynamic resistance and is calculated using a number of the vehicle's aerodynamic properties including drag coefficient, cross sectional area, length, inter-vehicle gap, number of bogies and number of pantographs (Rochard and Schmid, 2000). To simulate general aerodynamic changes, the existing c term is varied over ±5%.

Maximum Speed

The specified maximum speed is set as the line speed limit for the entire route. With the exception of coasting and braking phases, the vehicle is always trying to attain the maximum speed. The base value is set to a normal operational speed for the given service, and varied by ±20%.

Regeneration Use

To assess the impact of regeneration use a new variable is introduced into the simulator. The regeneration rate is set to be equal to the generation rate to simulate all regenerated power returning to the supply, minus the drive chain conversion losses. The new regeneration use variable then determines how much of the regenerated energy is actually used, i.e., the effective regeneration. It is varied from a base case of 0.5 by ±40%, so that effective regeneration ranges from 30% to 70%.

Coasting Phases

In the STS coasting phases can be introduced before all braking phases. Coasting refers to a mode during which no power is applied and the train decelerates purely due to resistive forces. When the train is preparing to stop, it first coasts until it reaches the specified coasting speed and then applies the brake (Figure 20). The lower the coasting limit, the shorter the braking phase but the longer the journey time. The base case for coasting is no coasting, i.e., the coasting limit is equal to the maximum speed. Coasting speed is then varied from 70% to 100% of maximum speed. This is the only factor for which the base case takes the maximum factor value. The factor values and their ranges are summarised in Tables 13 and 14, external factors are highlighted in grey.
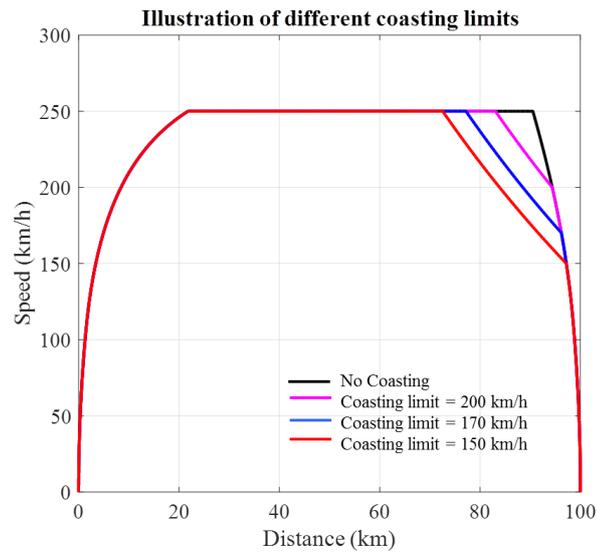
Figure 20: Example train trajectory when different coasting limits are specified

Table 13: Values and ranges for the factors which are unique to each subsystem

Network	Service	Line Length, km	Interstation Distance, km		Mass, t	Aerodynamics, Ns^2/m^3	Maximum Speed, km/h
		Fixed	Min	Max	(±10%)	(±5%)	(±20%)
Urban	Urban	30	0.7	2	108	0.007	70
Urban	Commuter	50	1	3	104	0.007	80
Inter-city	Commuter	60	3	20	105.8	0.004	120
Inter-city	High Speed	250	30	80	592.8	0.010	200
High Speed	Commuter	100	20	50	268.5	0.004	160
High Speed	High Speed	200	50	100	788.0	0.013	250

Table 14: Values and ranges for the factors which are the same across all subsystems

Factor	Base Case	Variation
Gradient	0	±0.01^c
Efficiency	0.85	±7%
Regeneration Use	0.5	±40%
Coasting Phases	Maximum Speed	-30%

6.3 Stage 6: Subsystem Results

The subsystem analysis aims to understand not only which factors are important, but the relationships between these factors and how they influence the KPIs. Firstly, the trends due to the external factors are evaluated by comparing the importance rankings of the factors. Then

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the key relationships between the factors are investigated using Principal Components Analysis (PCA) and data visualisation techniques. Scatter plots are primarily used as they provide a clear way of determining the trends due to individual factors. The PCA results indicate only the trends in terms of data variation and therefore do not necessarily reflect the importance of factors.

6.3.1 Urban Urban (UU)

Figure 21 shows the importance rankings for each value of the external factors, interstation distance and gradient, for the total energy and journey time KPIs for an Urban Urban subsystem. For energy, the most influential factors (in order of importance) are the coasting limit, maximum speed, efficiency and mass. Only for a steep uphill gradient does the ranking of factors change, with all of the influential factors converging in importance. Both coasting limit and maximum speed influence the journey time as would be expected, and mass also has a small impact. Consideration of both the μ* and σ values together for the energy KPI (Figure 22) indicates that all four influential factors have nonlinear or interaction effects with other factors (high μ*, high σ).

In order to better understand these relationships, PCA was performed on two datasets, each formed from the simulation run inputs and outputs from one Morris analysis. Each individual within each dataset has 8 variables, which are the values of the 6 input factors and the corresponding output values for energy and journey time. Because Morris evaluates trajectories of k+1 steps, the total number of individuals in each PCA is:

$$r(k + 1) = 560 \times 7 = 3,920$$
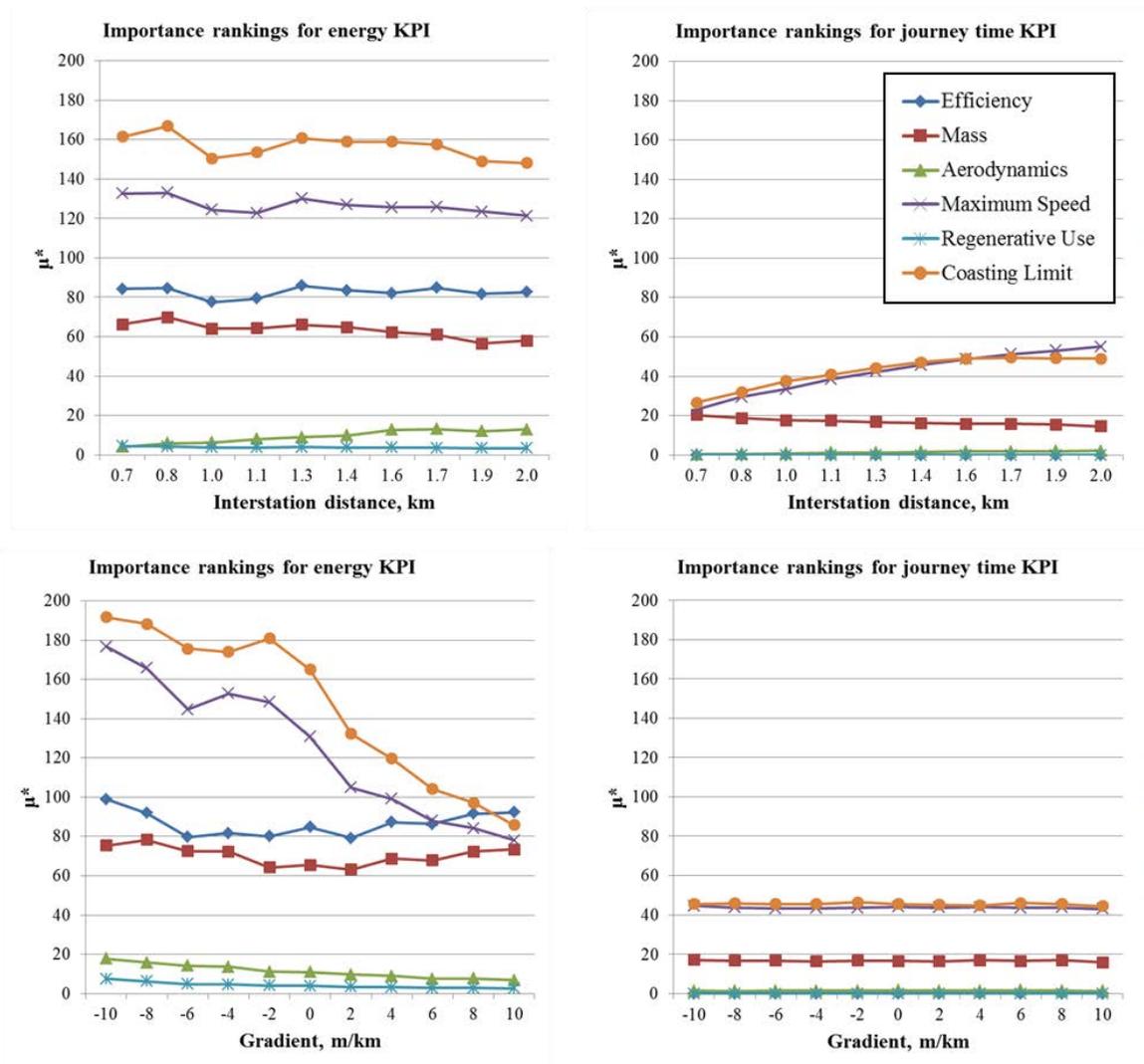
Figure 21: Importance rankings for all external factor values and KPIs for the UU subsystem
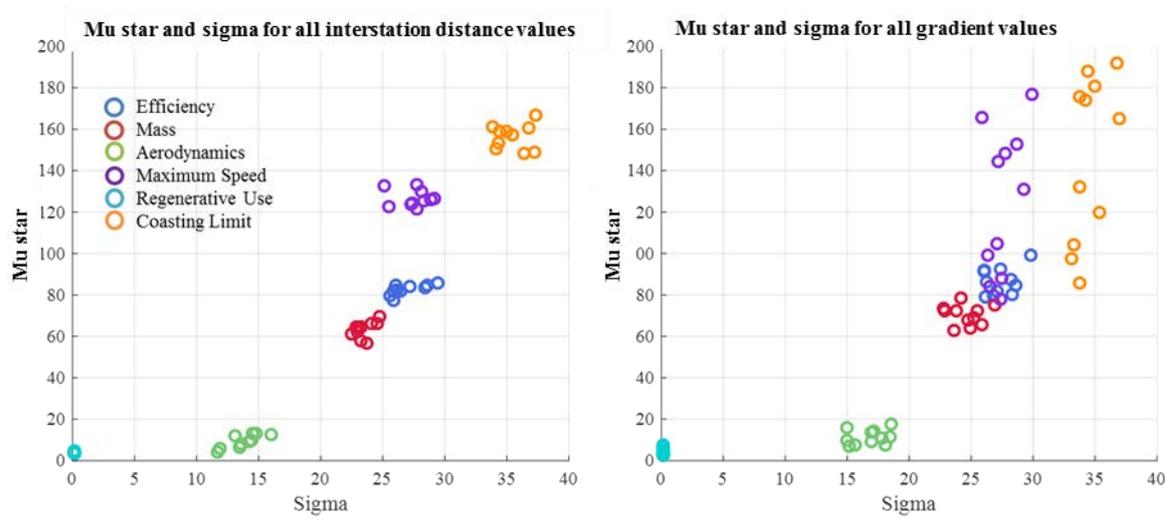
Figure 22: μ* against σ for all external factor values for the energy KPI for the UU subsystem

6.3.1.1 Analysis of interstation distance results

The first dataset analysed was the Morris evaluation when interstation distance was set to 2 km. This represents the general results for all interstation distance values, and the ranking for the majority of the gradient values too. The PCA shows that almost 90% of the total variation in the data is described by the first four PCs.
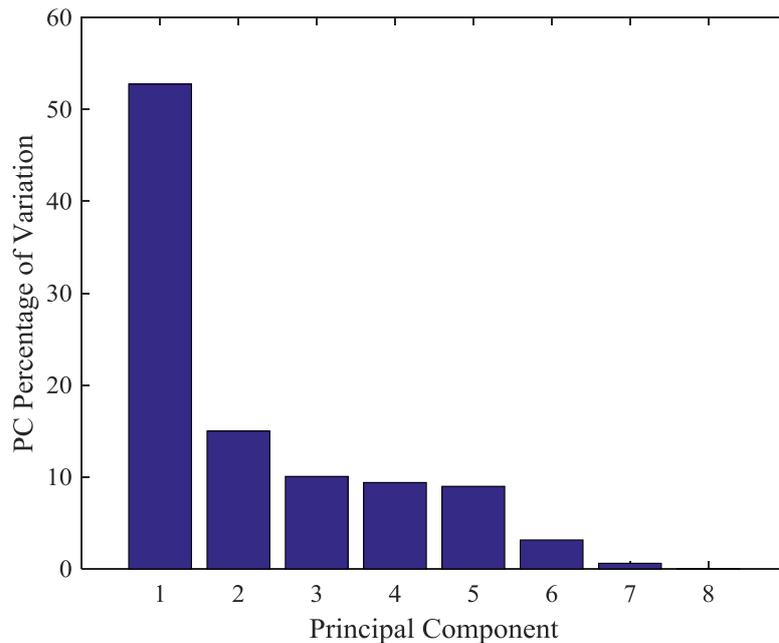
Figure 23: Percentage contribution of each PC to the total variation of the UU subsystem interstation distance dataset

Table 15 shows the PC scores for each of the first four Principal Components to 1 dp. Using a correlation value of 0.4, the red boxes show positive correlation and the blue boxes negative correlation. Choosing a correlation value is a subjective decision based on the data being analysed (Roths, 2016). In this case, 0.4 is chosen as a boundary value because it does not credit all factors with importance, nor does it discredit too many factors. The same value is applied to all subsystems to ensure consistency between the analyses. The scores are given to 1dp because in a number of cases the PC scores for factors are just below the 0.4 limit, e.g. 0.376, yet would still contribute to the results discussion. A correlation value to 2 dp could have been chosen to overcome this problem also, but I feel this would have made the results more difficult to read and interpret. When the PC scores are plotted, the non-rounded numbers from the PCA are used.

Looking at the PC scores for the UU interstation distance dataset, it can be deduced that only the first PC accounts for any significant variation in the energy and journey time variables. However, the remaining three PCs give an indication that relationships exist between the remaining factors.

Table 15: PC scores for UU subsystem with an interstation distance of 2km

	PC1	PC2	PC3	PC4
Efficiency	-0.2	0.5	-0.6	0.5
Mass	-0.2	0.5	0.6	-0.2
Aerodynamics	-0.2	0.4	0.3	0.4
Maximum Speed	-0.4	-0.2	-0.1	0.1
Regeneration Use	-0.2	0.4	-0.4	-0.8
Coasting Limit	-0.5	-0.2	0.0	0.0
Energy	-0.5	-0.2	0.2	-0.1
Journey Time	0.5	0.3	0.1	0.0

The key trend, shown by PC1, is that decreasing the maximum speed limit and the coasting limit (i.e., increasing the length of the coasting phase) decreases energy, but increases journey time. The second most important trend, shown by PC2, is that when all of the remaining factors are increased, they counterbalance each other, resulting in a minimal decrease in energy consumption and increase in journey time. In context this shows that the effectiveness of efficiency and regeneration improvements depends on the vehicle characteristics.

These two PCs can also be visualised using a bi-plot, as shown in Figure 24. In this representation the correlations between factors for each PC can be identified by looking at each axis independently. For example, the x-axis shows strong positive correlation between coasting limit, maximum speed and energy, and strong negative correlation between these factors and journey time. The y-axis on the other hand shows that positive values for efficiency, aerodynamics, mass and regen use only cause a relatively small increase in journey time and a small decrease in energy. The scatter shows the PC scores for each individual in the dataset. The regular shape and spacing indicates that the trajectories generated for the Morris analysis had good coverage of the search space.
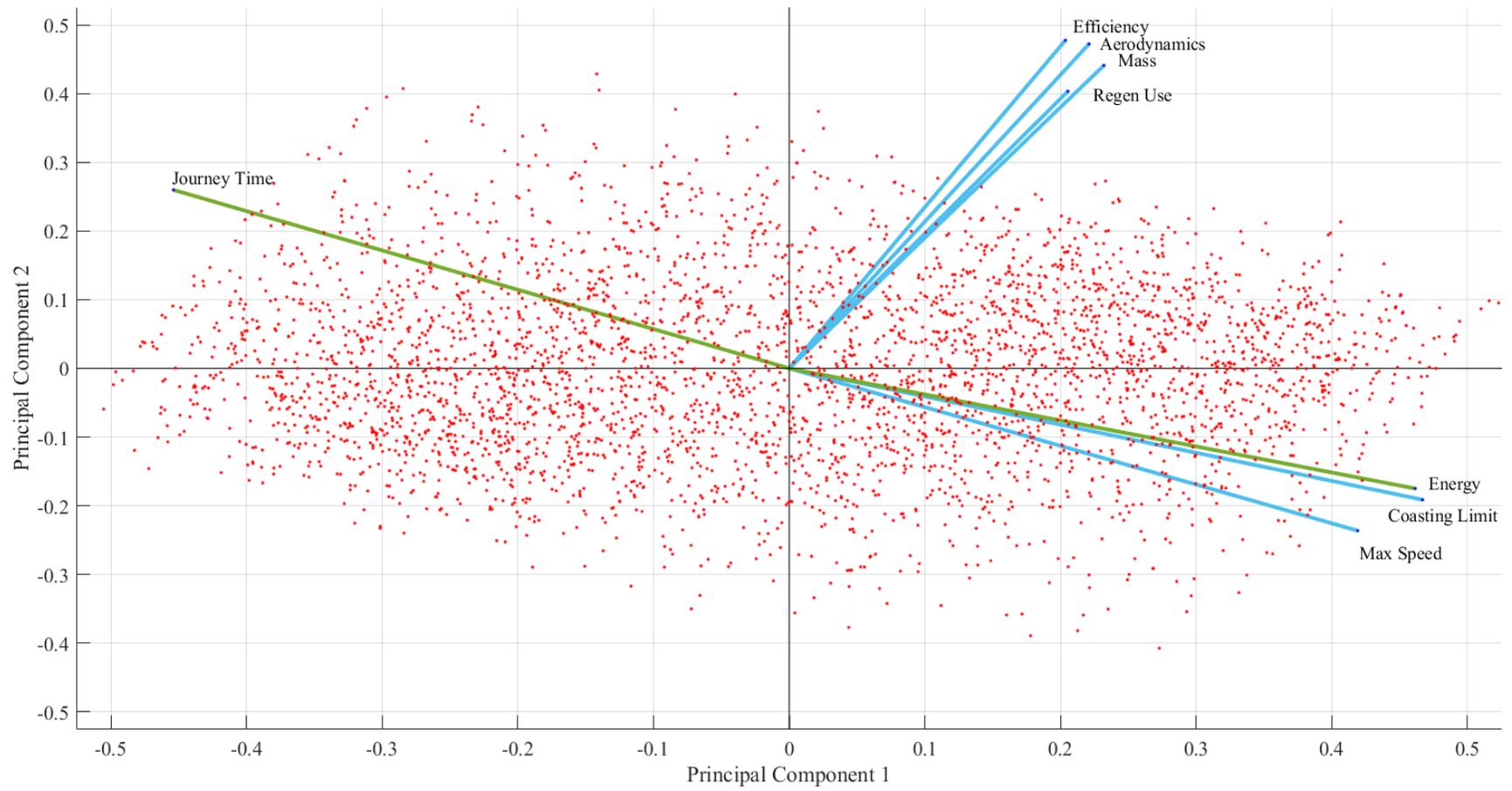
Figure 24: Bi-plot of PC1 and PC2 for the UU maximum interstation distance dataset

The PCA has shown that variation of the coasting limit and maximum speed variables has the greatest impact on journey time for an Urban service running on an Urban railway network. The remaining PCs indicate that the other four factors have strong interactions: particularly efficiency, which correlates with mass, regeneration use and aerodynamics. To ascertain that these observations are correct, the energy and journey time values for every individual have been plotted and then coloured according to the factor value of each of the important factors (Figure 25). This type of graph will henceforth be referred to as a 'Trend Identification Plot' or TIP.
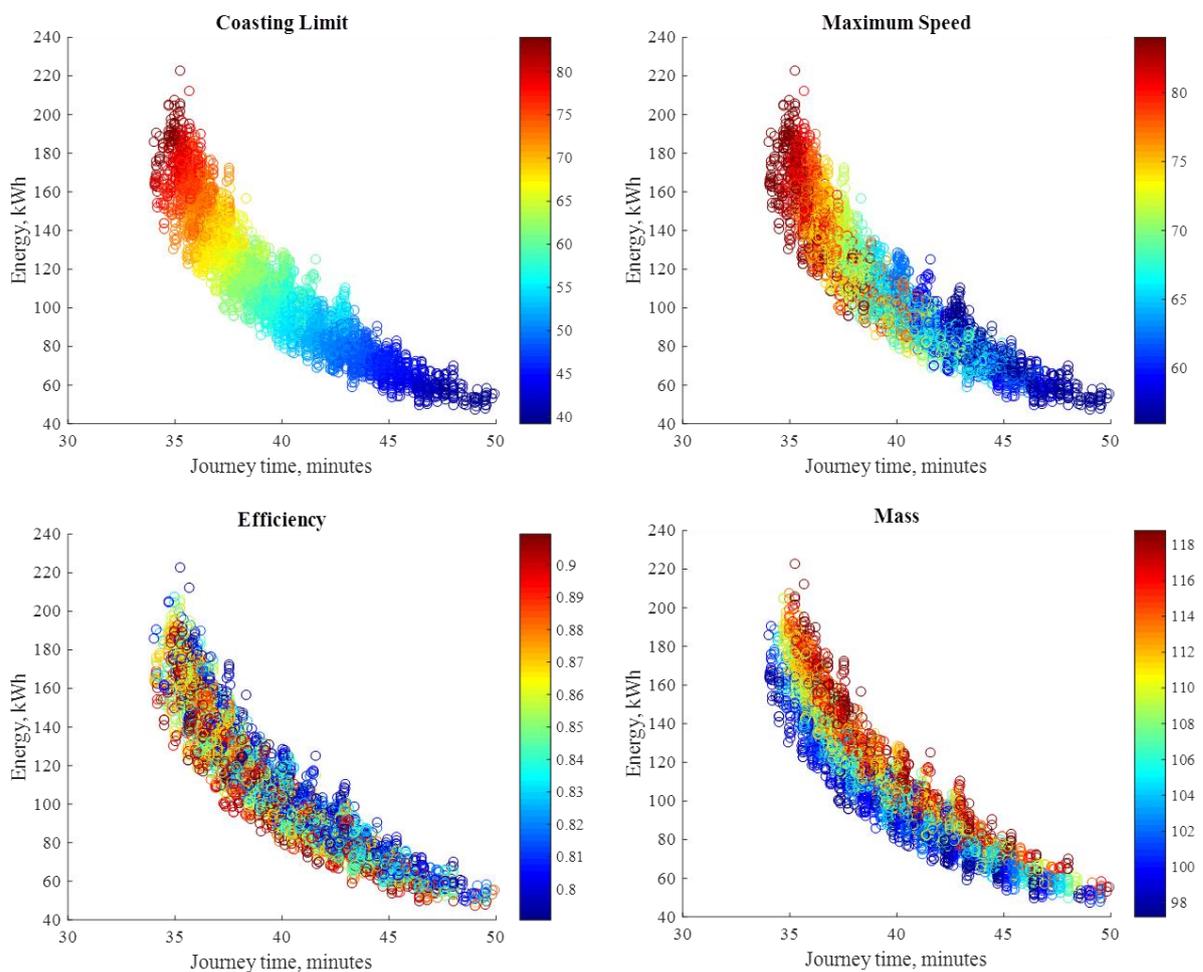
Figure 25: TIPs highlighting the relationships each of the four key factors have with energy and journey time, for the UU interstation distance dataset

The plots show that the coasting limit value directly influences the energy and journey time as identified in the PCA. The maximum speed shows a similar trend - high values generally result in a high energy consumption and low journey time – but the colour graduation is not as smooth meaning that maximum speed has some interaction with the other factors. The mass

graph displays a clear trend, whose implications are very interesting. The fact that high values sit at the top of the curve and low values at the bottom suggest that mass acts as a secondary optimisation variable. Although it cannot influence the overall energy and journey time in the same way as coasting limit and maximum speed, it is instead able to create local optima for a given set of values. This is demonstrated by Figure 26, which shows the TIP for mass, using only those individuals where the coasting limit is equal to the highest value of maximum speed (84 km/h).
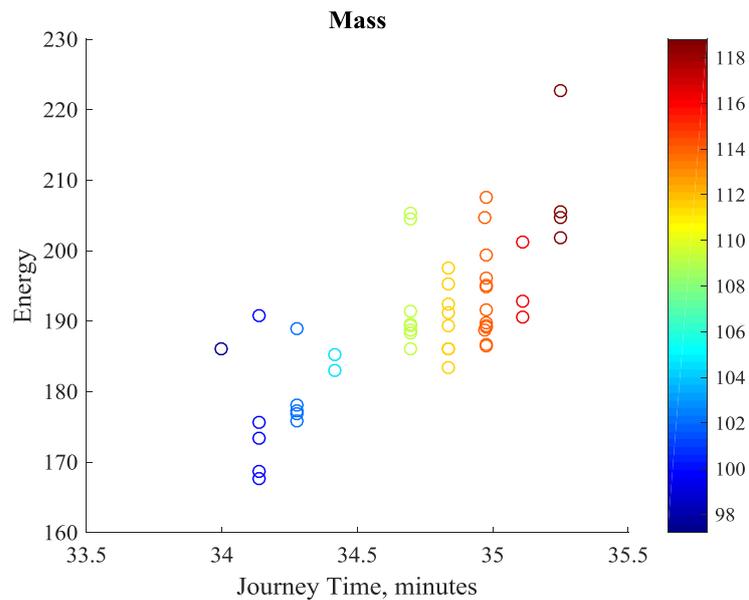
Figure 26: The correlation of mass with energy and journey time for UU subsystem individuals with coasting limit equal to 84 km/h

Efficiency displays a similar trend although the colour graduation is less distinct. Using the same individuals as for the previous figure, Figure 27 shows the same energy and journey time results coloured using the efficiency values. Although the trend appears very different, it shows that efficiency is also able to optimise energy locally. However, unlike mass, improving the efficiency has no impact on journey time, which accounts for the different colouring and the fuzzy appearance of the overall TIP.
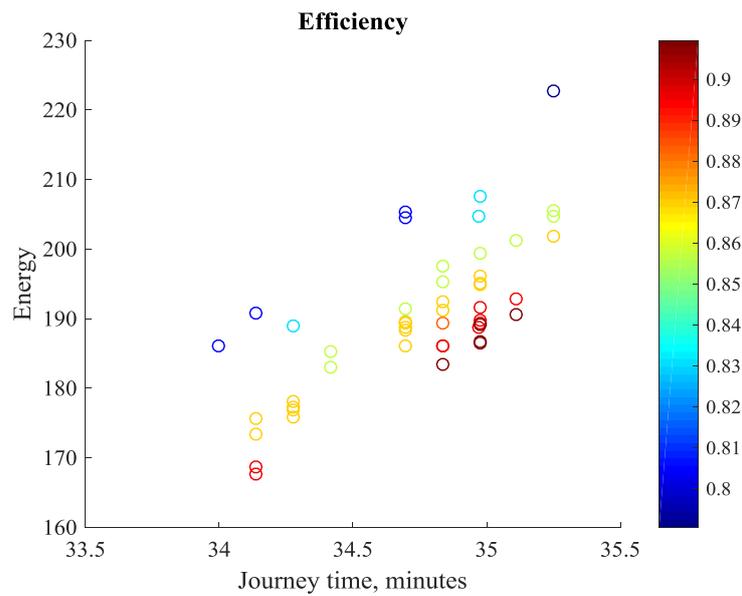
Figure 27: The correlation of efficiency with energy and journey time for UU subsystem individuals with coasting limit equal to 84 km/h

6.3.1.2 Analysis of gradient results

The second dataset analysed was where the Morris evaluation gradient was set to 10 m/km. The factor ranking only changes once the gradient exceeds 6m/km, and the importance of the top four factors appears to converge. PCA once again identified that four PCs account for 90% of the total variation, with over 50% attributable to PC1. The first two PCs are the same as the previous analysis indicating that the values of coasting limit and maximum speed have the greatest influence on energy consumption and journey time. The second two PCA are different. PC3 corroborates that mass and efficiency play a more important role when gradient increases. A high efficiency and reduced mass is able to reduce energy consumption, and marginally reduce journey time. A bi-plot of PC1 against PC3 is shown in Figure 28.

Table 16: PC scores for UU subsystem with a gradient of 10 m/km

	PC1	PC2	PC3	PC4
Efficiency	-0.2	0.4	0.7	0.4
Mass	-0.2	0.5	-0.5	0.4
Aerodynamics	-0.2	0.4	0.0	-0.8
Maximum Speed	-0.4	-0.3	0.1	0.0
Regeneration Use	-0.2	0.4	0.1	-0.1
Coasting Limit	-0.5	-0.1	0.0	0.0
Energy	-0.5	-0.1	-0.4	0.1
Journey Time	0.4	0.3	-0.2	0.0
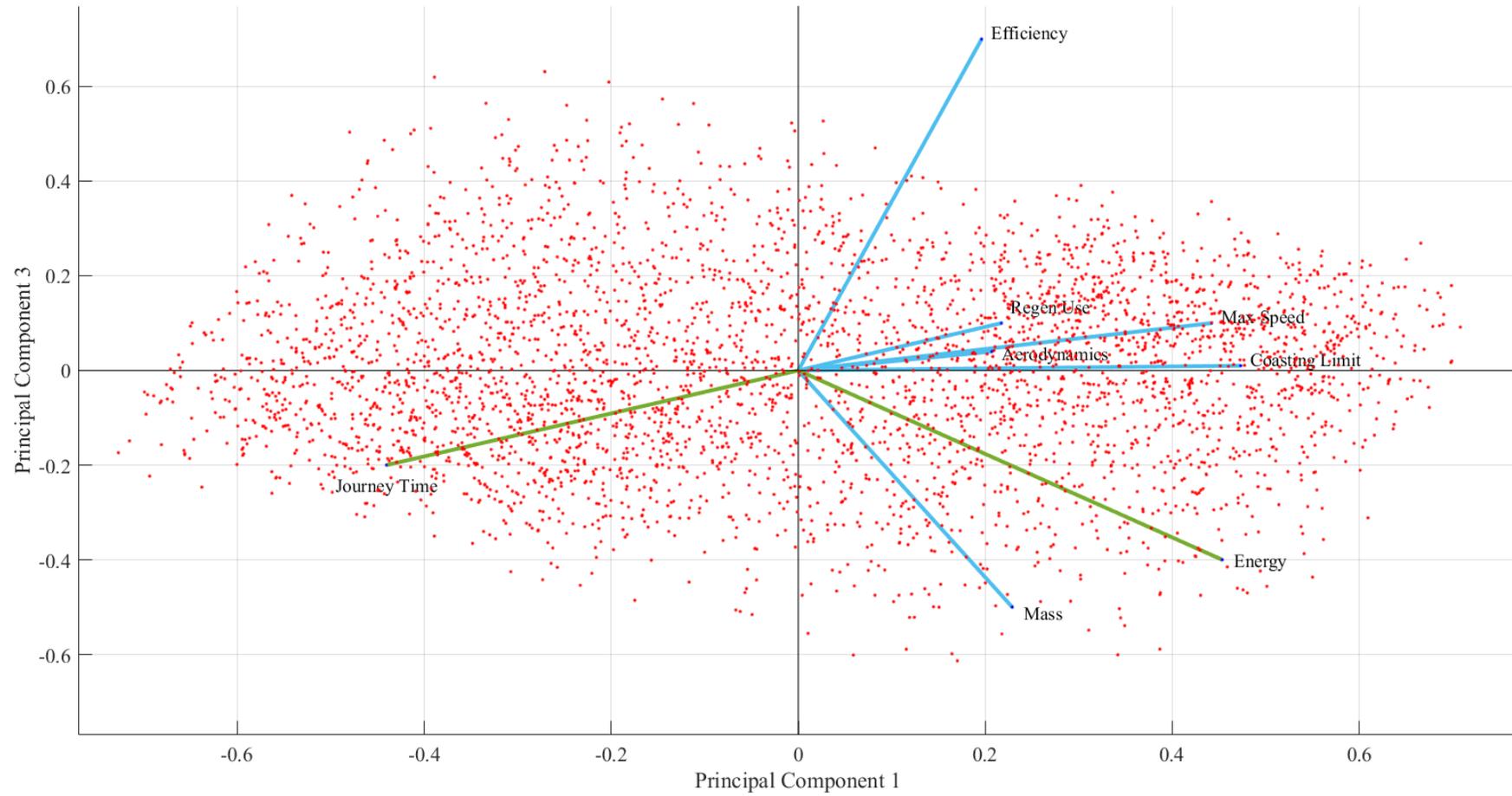
Figure 28: Bi-plot of PC1 and PC3 for UU subsystem with gradient of 10 m/km
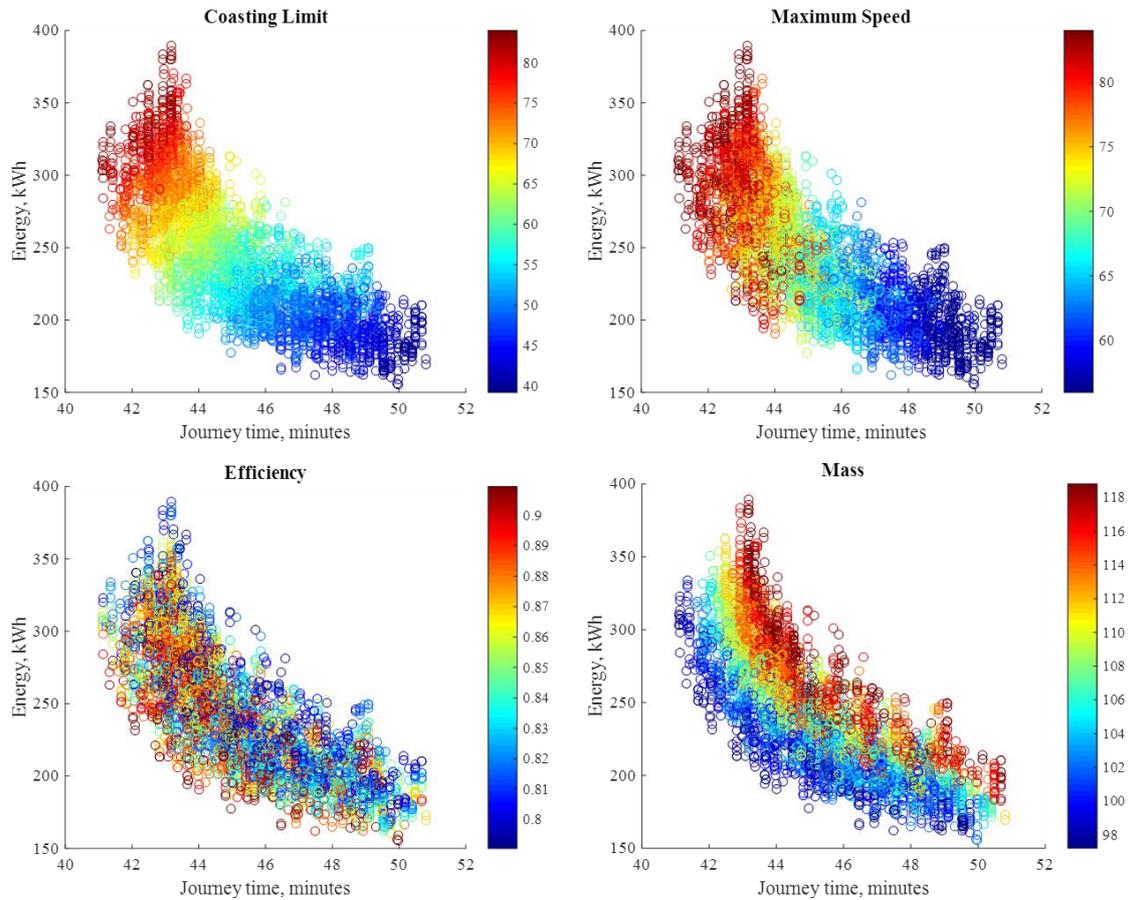
Figure 29: TIPs highlighting the relationships each of the four key factors have with energy and journey time, for the UU gradient dataset

The TIPs (Figure 29) confirm that the overall changes are minimal in terms of interaction relationships. The efficiency trend is much less clear than the previous results, which could be caused by increased interaction with other factors and the greater spread of energy and journey time values within this analysis.

6.3.2 Urban Commuter (UComm)

The importance rankings for the Urban Commuter subsystem are similar to those of the Urban Urban subsystem, as illustrated by Figure 30. The important factors are once again the coasting limit, maximum speed, efficiency and mass. A steep uphill gradient impacts the ranking order for energy, with the key factors appearing to converge. The influence of coasting limit on journey time drops off as the gradient increases, which suggests that it is less effective in these cases.
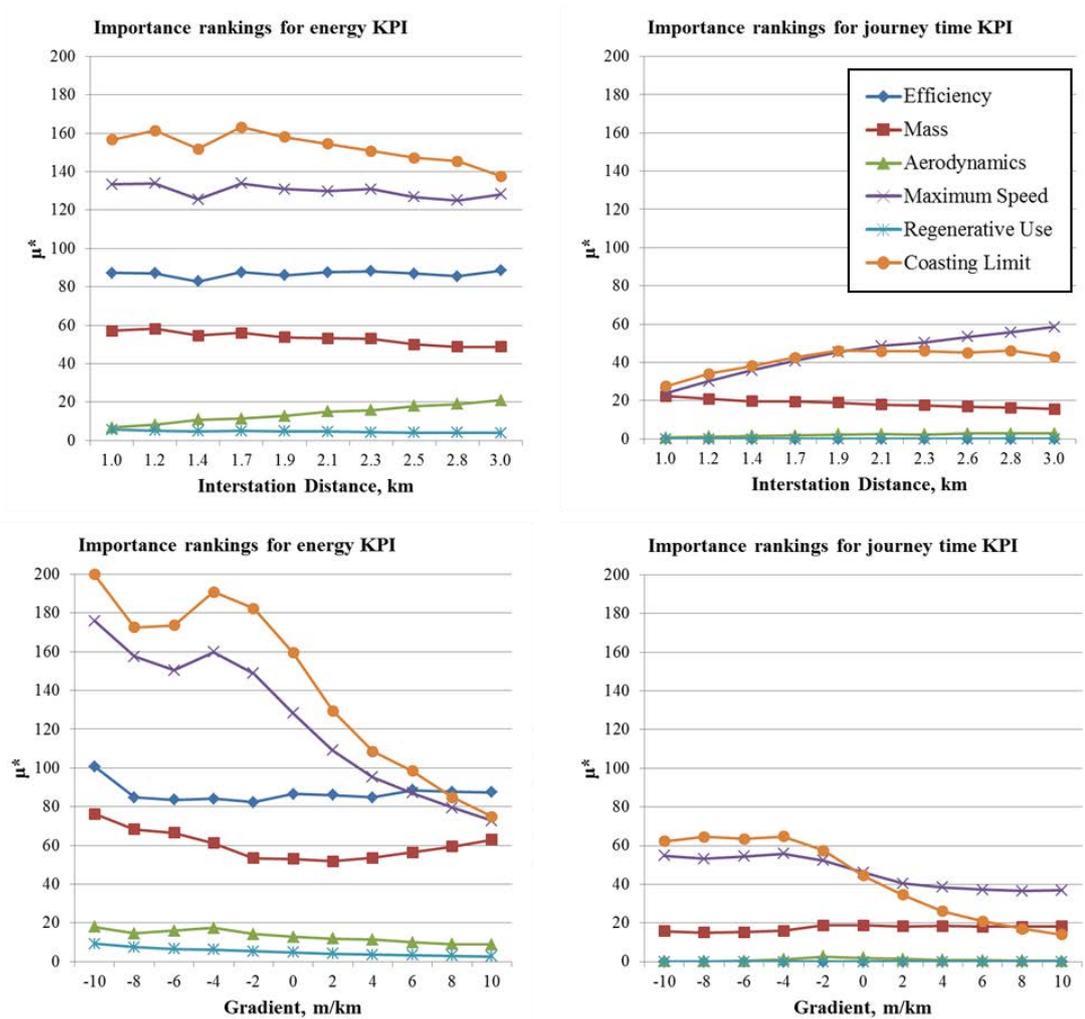
Figure 30: Importance rankings for all external factor values and KPIs for the UComm subsystem

The maximum interstation distance and maximum gradient were again chosen as datasets for PCA.

6.3.2.1 Analysis of interstation distance results

For a distance of 3 km, the PCA indicates that 90% of the variation is again attributable to the first four PC. The PC scores are extremely similar to those of the UU subsystem, with some minor changes which are specified in Table 17. Bold values show the difference from the UU subsystem scores, which are given in brackets. Green cells indicate a change from a significant value in the previous analysis to a non-significant value. The TIPs in Figure 31 show the trends previously identified, confirming the similarities between the UU and UComm subsystem results.

|	PC1	PC2	PC3	PC4
Efficiency	-0.2	0.5	**-0.4** (-0.6)	**-0.1** (0.5)
Mass	-0.2	**0.4** (0.5)	**0.8** (0.6)	**0.1** (-0.2)
Aerodynamics	-0.2	0.4	**-0.2** (0.3)	**0.8** (0.4)
Maximum Speed	-0.4	-0.2	**0.0** (-0.1)	**0.0** (0.1)
Regeneration Use	-0.2	**0.5** (0.4)	**-0.1** (-0.4)	**-0.7** (-0.8)
Coasting Limit	-0.5	-0.2	0.0	0.0
Energy	-0.5	-0.2	0.2	**0.0** (0.1)
Journey Time	0.5	**0.2** (0.3)	0.1	**0.0** (0.1)
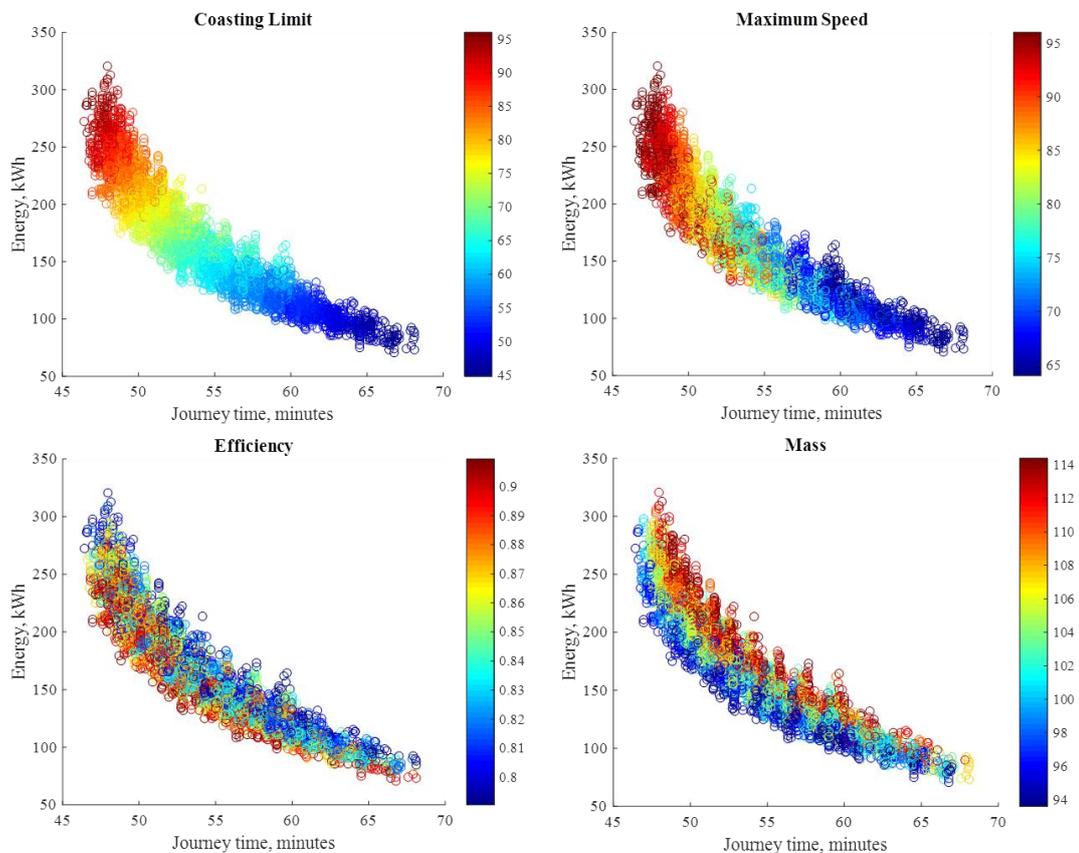
Figure 31: TIPs highlighting the relationships each of the four key factors have with energy and journey time, for the UComm interstation distance dataset

6.3.2.2 Analysis of gradient results

Using the same approach as for the interstation distance results, it has been confirmed that the Urban Commuter subsystem not only has the same importance rankings, but exhibits the same trends between factors as the Urban Urban subsystem. The percentage contribution of each PC, PC scores, bi-plot and TPIs are included in Appendix D for reference.

6.3.3 Inter-city Commuter (ICComm)

Figure 32 shows the importance rankings for the Inter-city Commuter subsystem. The $\mu*$ values indicate three factors of primary importance (coasting limit, maximum speed and efficiency), and two of secondary importance (mass and aerodynamics). However, these two levels are less distinct than for the previous subsystems. The effectiveness of the coasting limit depends on the distance between stations, dropping in importance as interstation distance increases. Aerodynamics, on the other hand, increases in importance relative to the interstation distance.
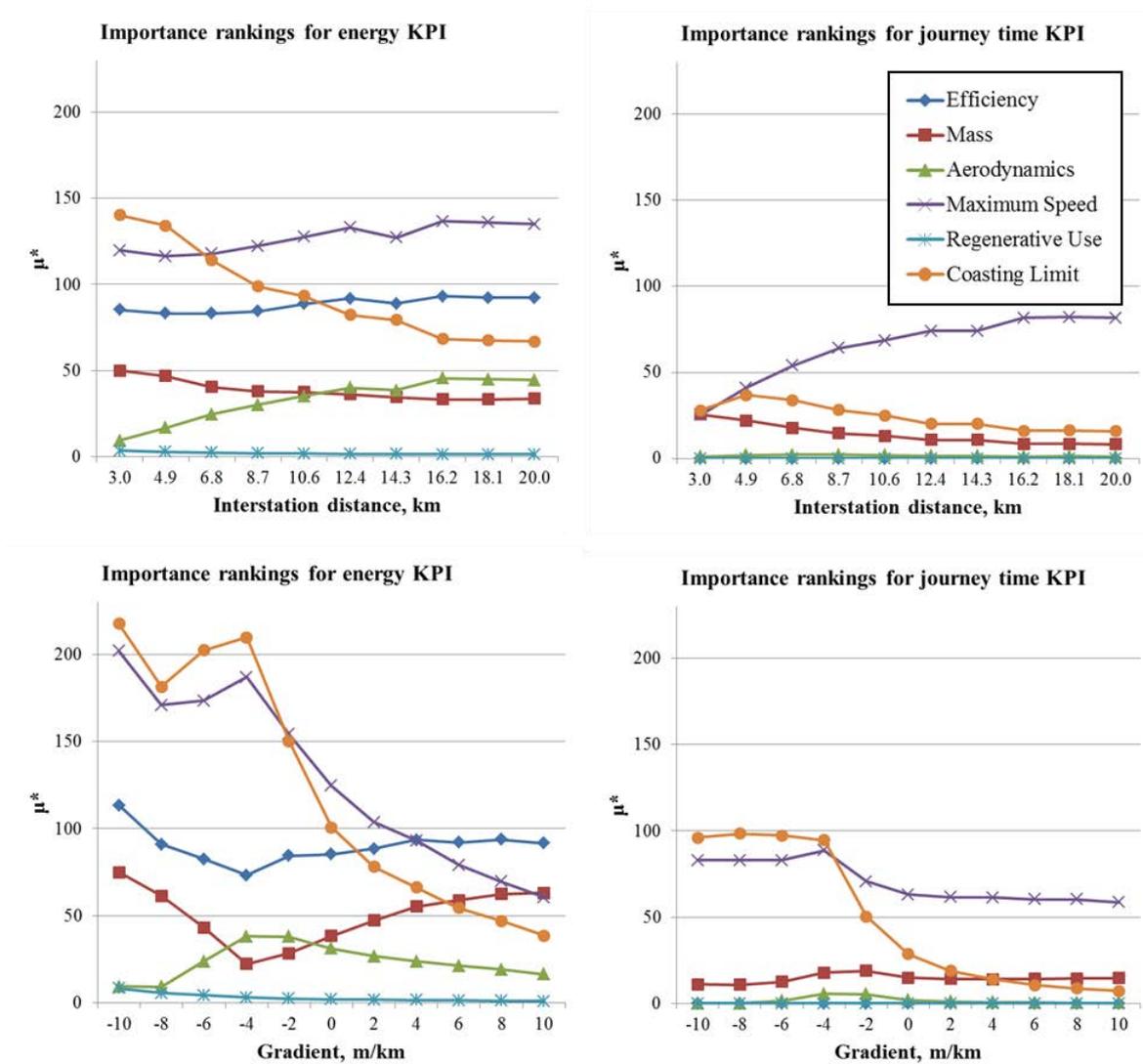
Figure 32: Importance rankings for all external factor values and KPIs for the ICComm subsystem

As with the previous subsystems, uphill gradients reduce the importance of both maximum speed and coasting limit, meaning that the importance of factors appears to converge.

However, in this instance, the importance of mass and aerodynamics does not remain consistent across all gradient values but instead dips and peaks around -4 m/km.

To better understand the changing relationships that are indicated by the results, three datasets were chosen for the PCA. The first two datasets were evaluated at the minimum and maximum values of interstation distance, in order to explore the impact this has on factor trends. The third, as done previously, was taken at the maximum uphill gradient. For downhill gradients the results are the same as the general results from previous analyses: coasting limit and maximum speed have the greatest impact on energy.

3.3.1 Analysis of interstation distance results

For both the minimum and maximum values of interstation distance, the first PC accounts for approximately 50%, and the first four for just under 90% of the total variance. However, although the scores for PC1 match the previous analyses, the remaining PCs indicate some slight differences in the factor relationships. The scores for the minimum and maximum values of interstation distance, in comparison to the UComm subsystem interstation distance results, are shown in Tables 18 and 19 respectively. In addition to green cells, which show a change from a significant to a non-significant value, the purple cells indicate a change from a non-significant to a significant value, and orange cells represent a change of sign for a significant factor.

For the minimum interstation distance value, PC2 represents the relationship between mass and journey time, which is indicated in the Morris importance rankings for journey time but not incorporated in PC1. The change in efficiency and regeneration can have no impact on journey time due to the simulator programming, so their high values in this case indicate their ability to counterbalance the energy increase caused by making vehicles heavier and less aerodynamic.

PCs 3 and 4 are different for each of the interstation distance datasets, implying that the trends between factors will be different in each case. These are explored further using TIPs.

	PC1	PC2	PC3	PC4
Efficiency	-0.2	**0.4** (0.5)	**0.5** (-0.4)	**0.1** (-0.1)
Mass	-0.2	**0.5** (0.4)	**-0.7** (0.8)	**0.0** (0.1)
Aerodynamics	-0.2	**0.3** (0.4)	0.2 (-0.2)	**-0.8** (0.8)
Maximum Speed	-0.4	-0.2	-0.1 (0.0)	0.0
Regeneration Use	-0.2	0.5	0.2 (-0.1)	**0.6** (-0.7)
Coasting Limit	-0.5	**-0.1** (-0.2)	**-0.1** (0.0)	0.0
Energy	-0.5	-0.2	**-0.2** (0.2)	0.0
Journey Time	**0.4** (0.5)	0.4 (0.2)	**-0.2** (0.1)	0.0

Table 19: PC scores for ICComm subsystem with an interstation distance of 20 km

	PC1	PC2	PC3	PC4
Efficiency	-0.2	**0.6** (0.5)	**0.1** (-0.4)	**0.1** (-0.1)
Mass	-0.2	0.4	**-0.7** (0.8)	**0.5** (0.1)
Aerodynamics	-0.2	0.4	**0.7** (-0.2)	**0.3** (0.0)
Maximum Speed	-0.4	-0.2	0.0	0.0
Regeneration Use	-0.2	**0.4** (0.5)	**-0.2** (-0.1)	**-0.8** (-0.7)
Coasting Limit	-0.5	**-0.1** (-0.2)	0.0	0.0
Energy	-0.5	-0.2	**0.0** (0.2)	**0.1** (0.0)
Journey Time	0.5	0.2	**0.0** (0.1)	0.0

Minimum Interstation Distance

Figure 33 shows the TIPs for minimum interstation distance. The trend between coasting limit, energy and journey time is immediately distinct, likewise is that of mass as a secondary optimisation variable (such as in the UU subsystem analysis). Although there is a linear trend between maximum speed, energy and journey time, the lack of distinct graduation indicates some interaction with other variables. Based on the PCA, this was likely to be the coasting limit, which is confirmed in Figure 34. Identifying the trend for efficiency is somewhat more challenging. There appears to be a linear trend for only the very highest energy values, which was confirmed by plotting those individuals with an energy result above 500 kWh and those below 200 kWh separately in Figure 35.
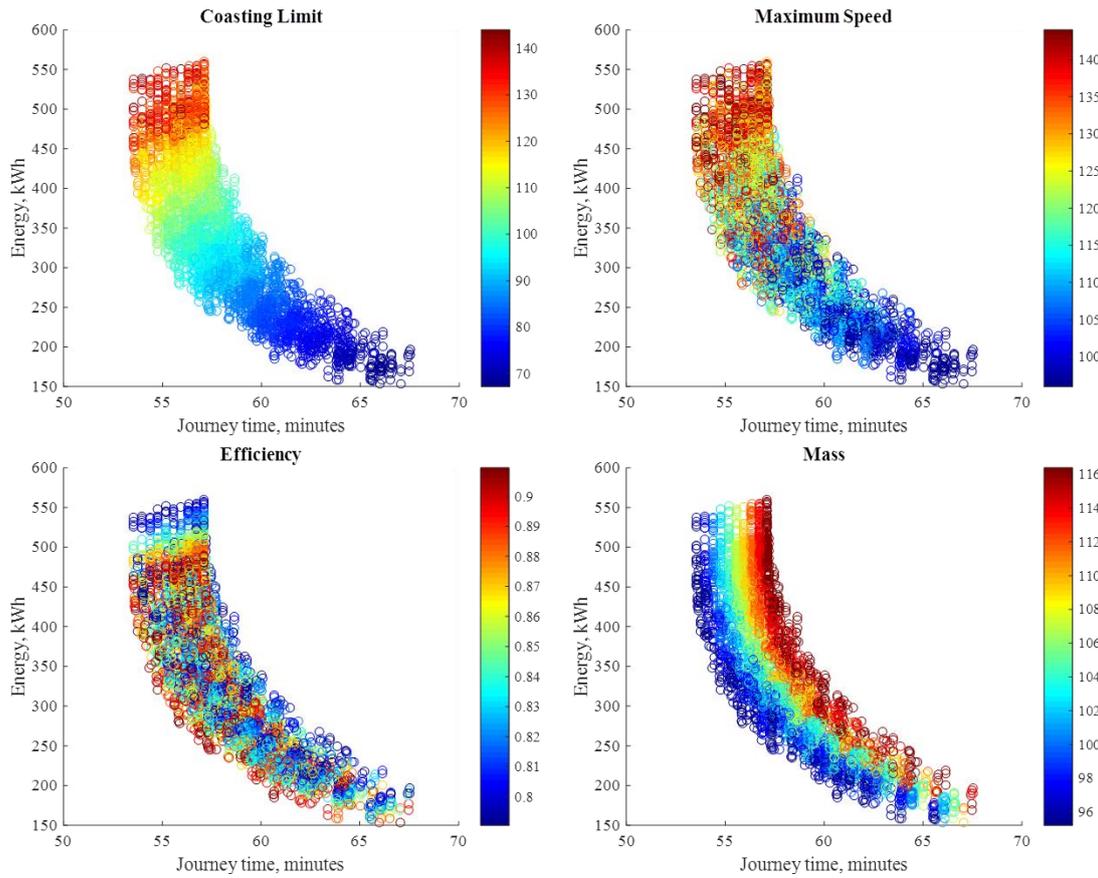
Figure 33: TIPs highlighting the relationships each of the four key factors have with energy and journey time, for the ICComm minimum interstation distance dataset
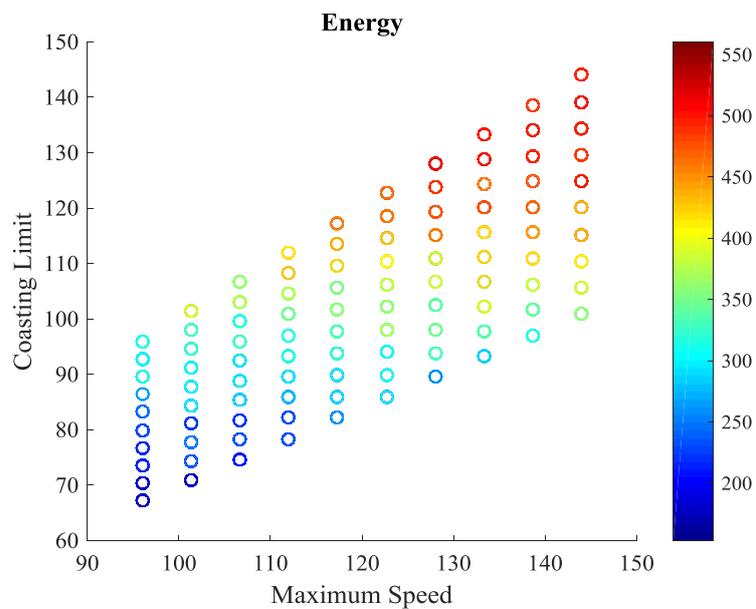
Figure 34: The correlation of energy with coasting limit and maximum speed for ICComm minimum interstation distance dataset
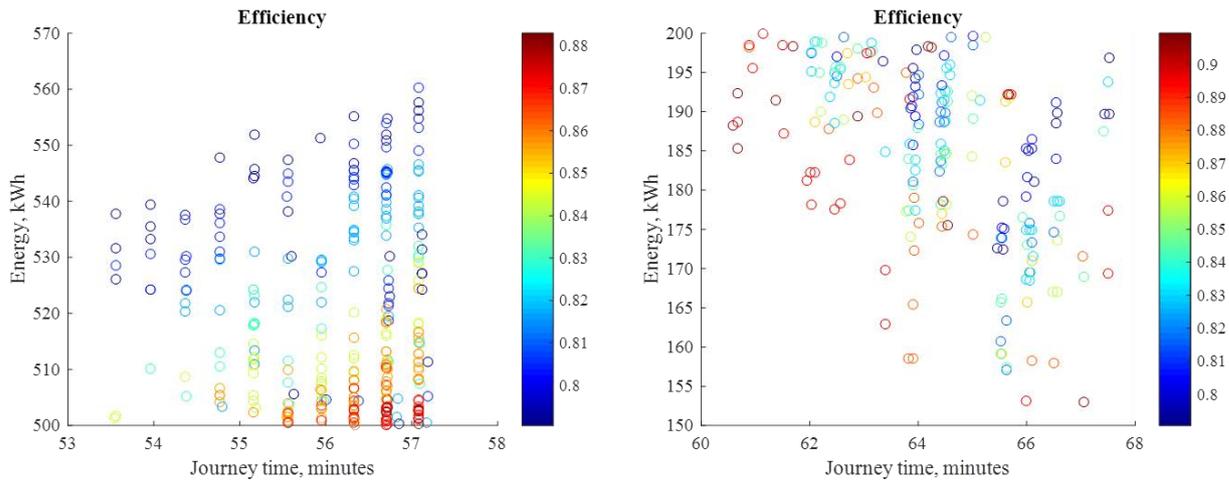
Figure 35: The correlation of efficiency with energy and journey time for ICComm minimum interstation distance energy results above 500 kWh (left) and below 200 kWh (right)

There is a clear pattern in the left hand graph but it is much more difficult to describe a trend in the right hand graph, which points to interactions. Within the UU subsystem analysis a relationship between coasting limit, mass and efficiency was indicated. Applying this knowledge and generating a plot of these factors reveals such a trend, as illustrated in Figure 36, which cannot be seen when each pair of variables is plotted separately (Figure 37).
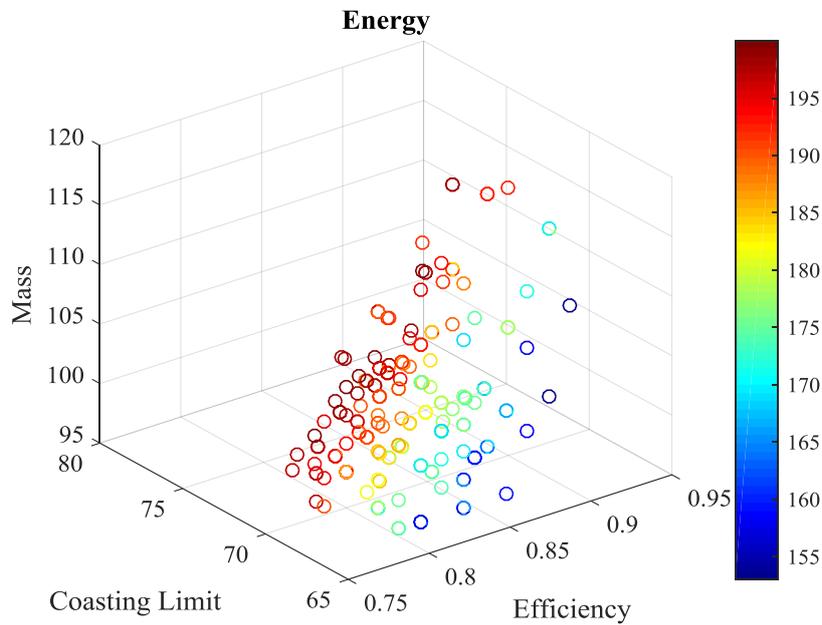
Figure 36: The correlation between energy, mass, coasting limit and efficiency for ICComm minimum interstation distance results with energy below 200 kWh

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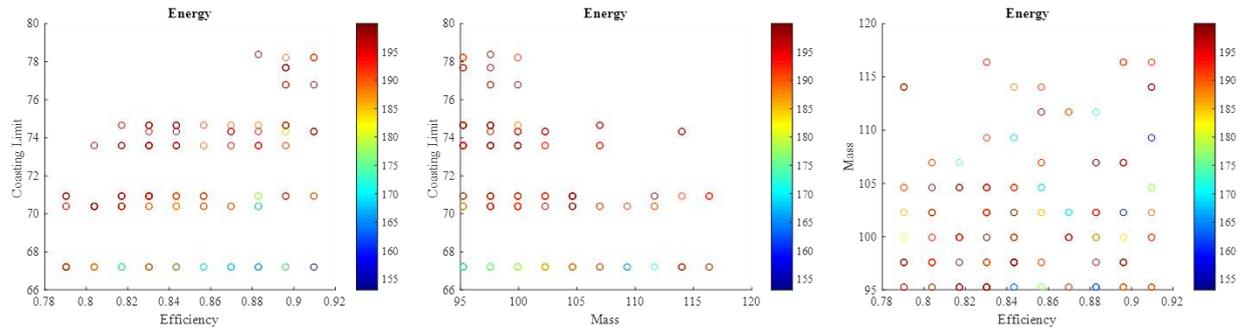
Figure 37: The correlation between energy, coasting limit and efficiency (left); energy, coasting limit and mass (middle) and energy, mass and efficiency (right); for ICComm minimum interstation distance results with energy below 200 kWh

Maximum Interstation Distance

Based on the colour graduation of the TIPs of maximum speed and coasting limit (Figure 39), it can be determined that, although they are both important primary factors, maximum speed has a greater influence on energy and journey time. As in previous analyses, mass and efficiency display trends that suggest local optimisation. This is confirmed in Figure 38, which shows similar trends to the UU subsystem analysis that have been highlighted by considering one isolated group based on the variables maximum speed and coasting limit. The trend for efficiency is much clearer in the TIP, which is likely attributable to its increased importance.
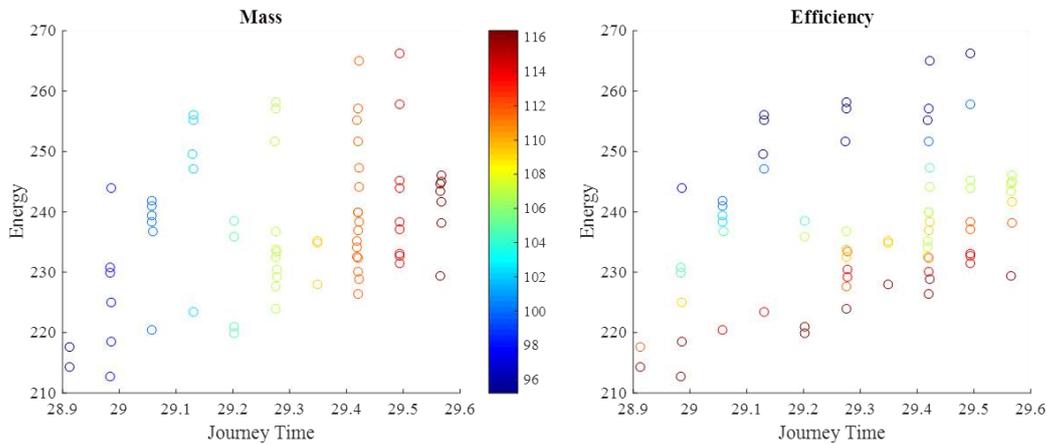
Figure 38: The correlation of mass and efficiency with energy and journey time for ICComm subsystem individuals with coasting limit equal to 144 km/h (maximum)

Aerodynamics is also included in Figure 39 due to its high importance. The result suggests that aerodynamics has a linear trend but significantly interacts with a number of different factors. Based on the PCA, these could be efficiency, mass, and regeneration use. However,

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the trend will also be influenced by the coasting limit and maximum speed, meaning that the impact aerodynamics has depends on the values of all of the other factors.
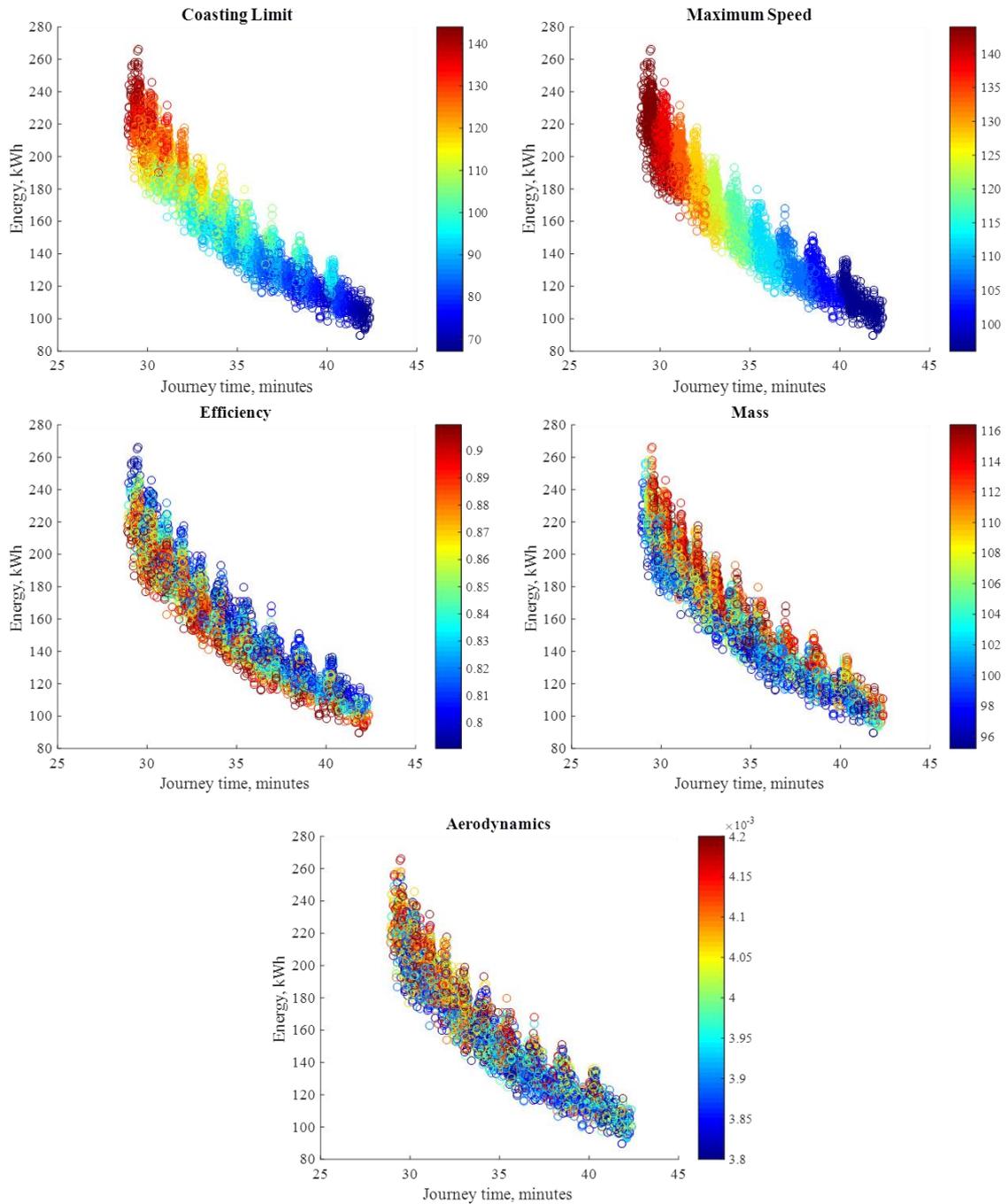
Figure 39: TIPs highlighting the relationships each of the four key factors have with energy and journey time, for the ICComm maximum interstation distance dataset

3.3.2 Analysis of gradient results

Although the order of factor importance for the ICComm subsystem is different to the order for the Urban network analyses, the PCA of the dataset for a gradient of 10 m/km indicated similar factor relationships to those previously found. The key factors were once again efficiency, mass, maximum speed and coasting limit. Table 20 shows the PC scores compared with those of the UU maximum gradient dataset. Even though the PC scores are not beyond the threshold of significance, it is worthwhile to note that the increased importance of efficiency and mass in terms of energy and journey time variation is reflected in PC3.

Table 20: PC scores for ICComm subsystem with a gradient of 10 m/km

	PC1	PC2	PC3	PC4
Efficiency	-0.2	**0.6** (0.4)	**-0.5** (0.7)	**-0.5** (0.4)
Mass	-0.2	**0.3** (0.5)	**0.7** (-0.5)	**-0.4** (0.4)
Aerodynamics	-0.2	0.4	**0.2** (0.0)	**0.5** (-0.8)
Maximum Speed	**-0.5** (0.4)	**-0.2** (-0.3)	**-0.2** (0.1)	**-0.1** (0.0)
Regeneration Use	-0.2	0.5 **(0.4)**	**-0.1** (0.1)	**0.5** (-0.1)
Coasting Limit	-0.5	-0.1	**-0.1** (0.0)	0.0
Energy	**-0.4** (-0.5)	**-0.2** (-0.1)	**0.3** (-0.4)	**0.0** (0.1)
Journey Time	0.4	0.3	**0.3** (-0.2)	0.0

The TIPs showed similar relationships to previous analyses. The percentage contribution of each PC, bi-plot and TIPs are included in Appendix D for reference.

6.3.4 Inter-city High Speed (ICHS)

The importance rankings, shown in Figure 40, indicate that the key factors are maximum speed and efficiency. Coasting limit and aerodynamics also have some impact, but mass is no longer an important factor for interstation distance. However, it does become significant if the route gradient is steep. Coasting can also be used effectively if there is a steep downhill gradient.

The PCA analysis datasets were chosen as the middle interstation distance (57.8 km) and maximum gradient to evaluate the relationships between factors.
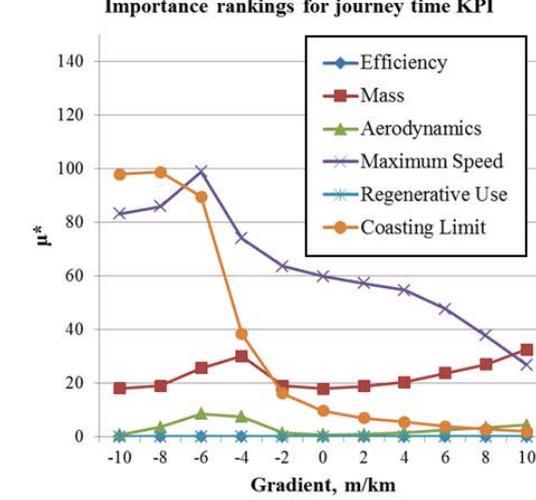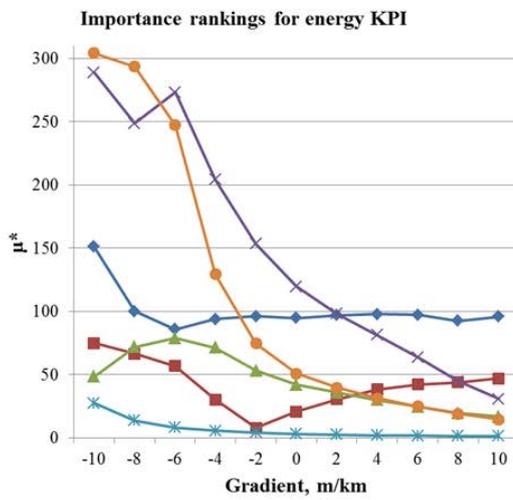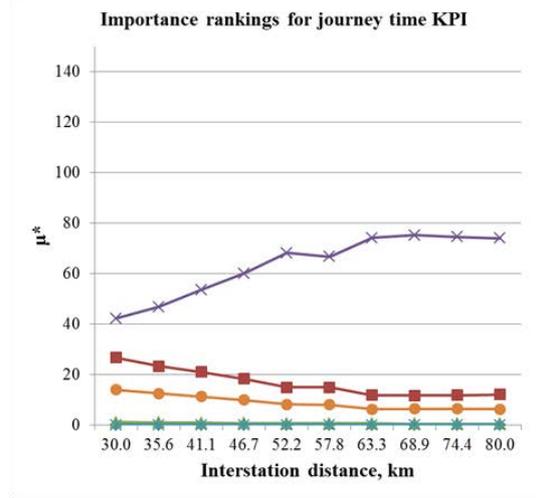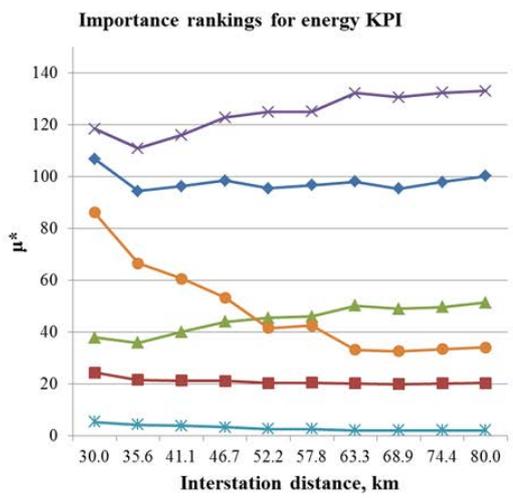
Figure 40: Importance rankings for all external factor values and KPIs for the ICHS subsystem

3.4.1 Analysis of interstation distance results
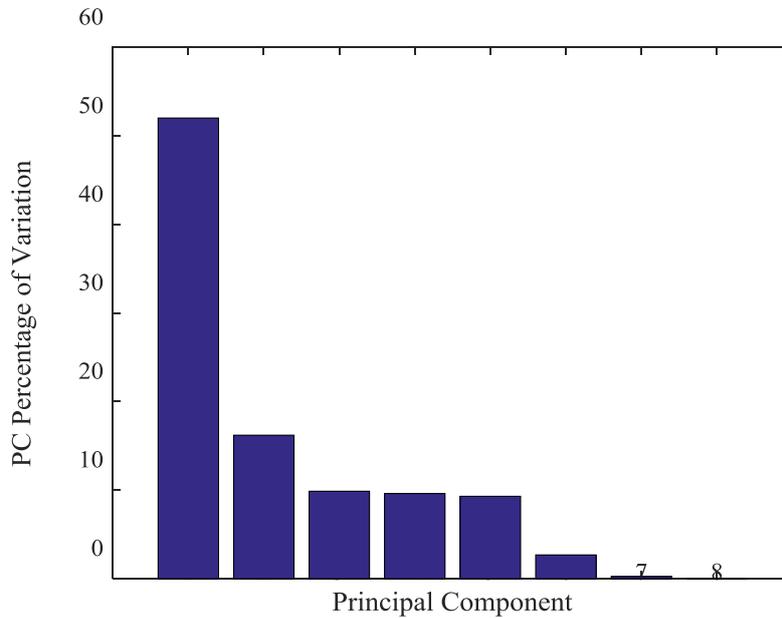
Figure 41: Percentage contribution of each PC to the total variation of the ICHS subsystem interstation distance dataset

The interstation distance results indicate similar relationships between factors as the previous analyses. Over 50% of the dataset variation is attributable to PC1 (Figure 41), which indicates that energy can be saved by reducing the maximum speed and implementing coasting, but that this increases journey time. Using the scores in Table 21, PC2 once again highlights a relationship between efficiency, mass, aerodynamics and regeneration use. However, the only key factor here, as determined by the Morris SA, is efficiency. The remaining variation in PC3 and PC4 is due to mass and regeneration use, and aerodynamics and regeneration use respectively. The TIPs (Figure 42) show clear relationships between energy and journey time for maximum speed, efficiency and coasting limit, which agree with previous analyses. Although aerodynamics has some colour graduation, its lack of distinction means it strongly interacts with other factors.

Table 21: PC scores for Inter-city High Speed subsystem with an interstation distance of 57.8 km

	PC1	PC2	PC3	PC4
Efficiency	-0.2	0.5	0.1	-0.3
Mass	-0.2	0.4	-0.9	0.0
Aerodynamics	-0.2	0.4	0.3	0.8
Maximum Speed	-0.5	-0.2	0.0	-0.1
Regeneration Use	-0.2	0.4	0.4	-0.4
Coasting Limit	-0.5	-0.1	0.0	0.0
Energy	-0.5	-0.2	-0.1	0.1
Journey Time	0.5	0.3	-0.1	0.1
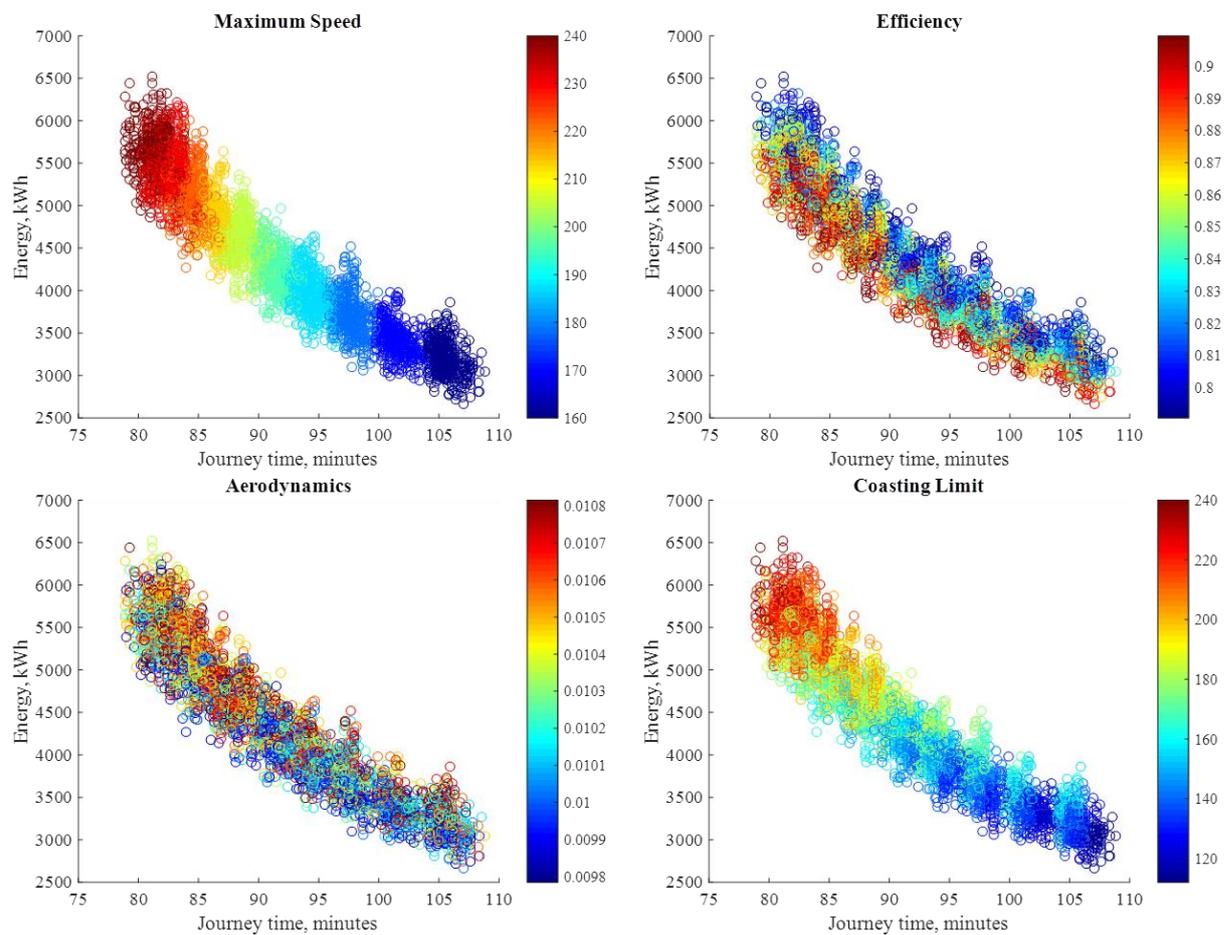
Figure 42: TIPs highlighting the relationships each of the four key factors have with energy and journey time, for the ICHS interstation distance dataset

3.4.2 Analysis of gradient results

Although the PC1 scores (Table 22) show the same relationship as the other analyses, the PC2 and PC3 scores indicate that other factors have more an effect on energy and journey time

than in the previous tests. The percentage of the total variation accounted for by PC1 has dropped by approximately 10% compared to the other tests and those for PC2 and PC3 have increased by roughly 5% each (Figure 43).
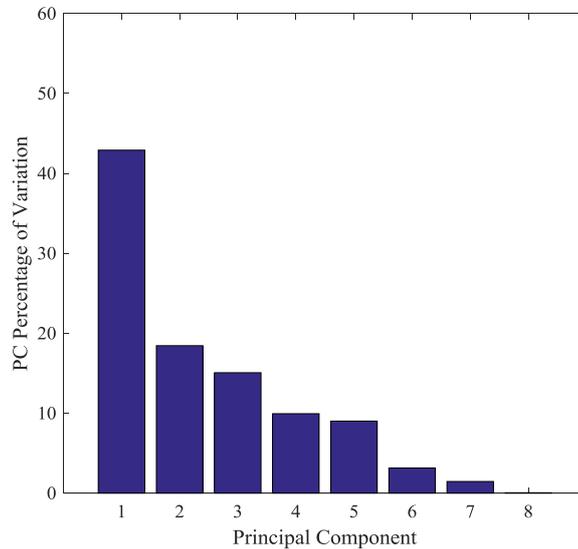
Figure 43: Percentage contribution of each PC to the total variation of the ICHS subsystem gradient dataset

Table 22: PC scores for ICHS subsystem with a gradient of 10 m/km

|	PC1	PC2	PC3	PC4
Efficiency	-0.2	0.6	-0.4	-0.2
Mass	-0.3	0.3	0.7	-0.2
Aerodynamics	-0.2	0.4	0.0	0.9
Maximum Speed	-0.5	-0.1	-0.1	-0.1
Regeneration Use	-0.2	0.4	0.0	-0.4
Coasting Limit	-0.5	0.0	-0.1	-0.1
Energy	-0.4	-0.3	0.4	0.1
Journey Time	0.4	0.4	0.4	0.0

PC2 indicates a strong relationship between efficiency, aerodynamics, regeneration use, and journey time. PC3 reflects the increased importance of efficiency and mass in line with the Morris SA results (Figure 40 shows the first distinct instance that maximum speed and coasting limit are not one of the two most important factors for maximum gradient). Figure 45 (overleaf) is a bi-plot of PC2 and PC3, which clearly demonstrates the importance of efficiency and mass. The TIPs in Figure 44 show strong relationships for mass, efficiency and

maximum speed with energy and journey time. However, the influence of the coasting limit is noticeably weaker than for previous analyses, which correlates with its decreased importance. No pattern is discernable for aerodynamics. However, the μ* value at this point indicates it has minimal impact.
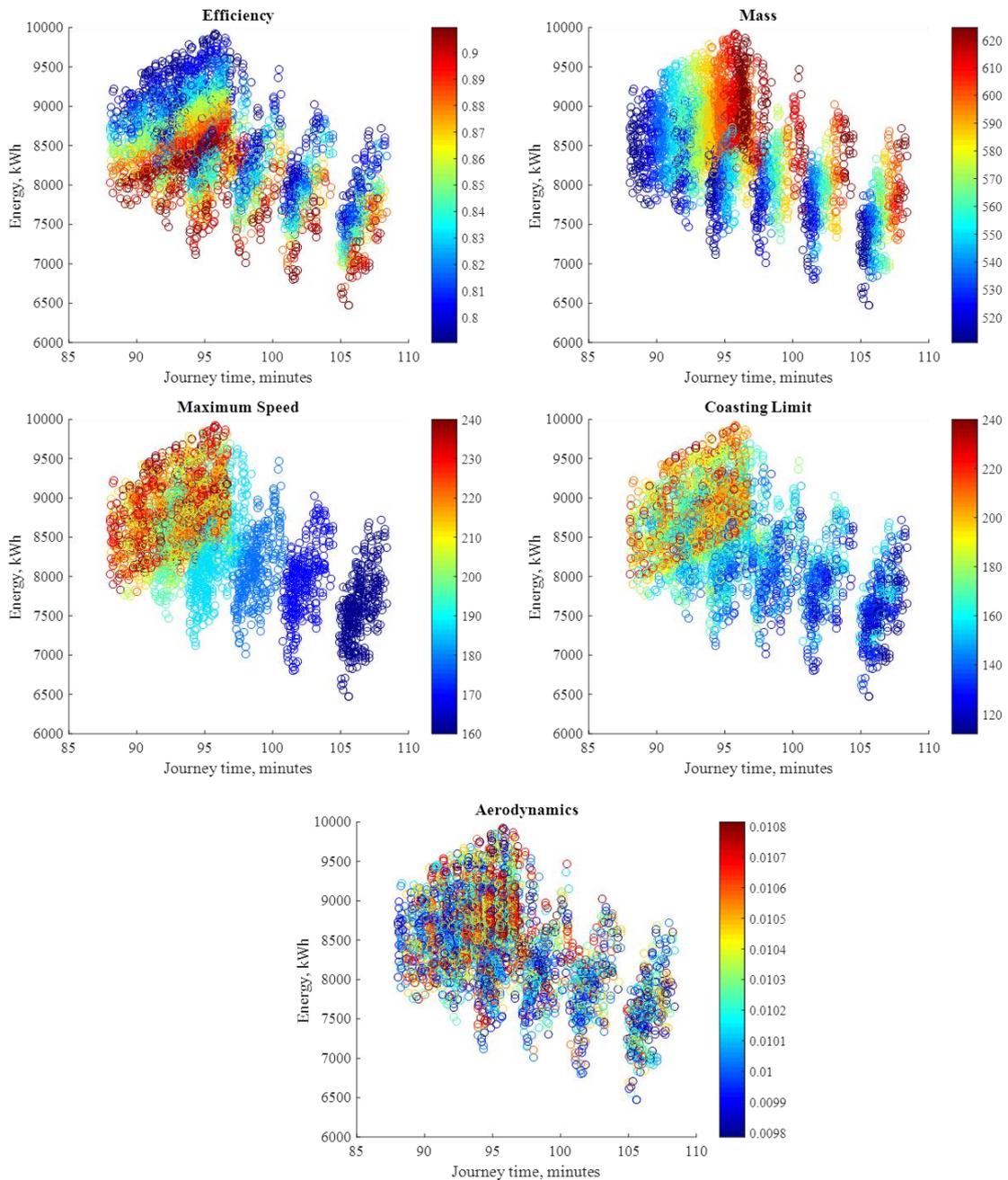
Figure 44: The correlation of the top five factor values with energy and journey time for ICHS subsystem maximum gradient dataset
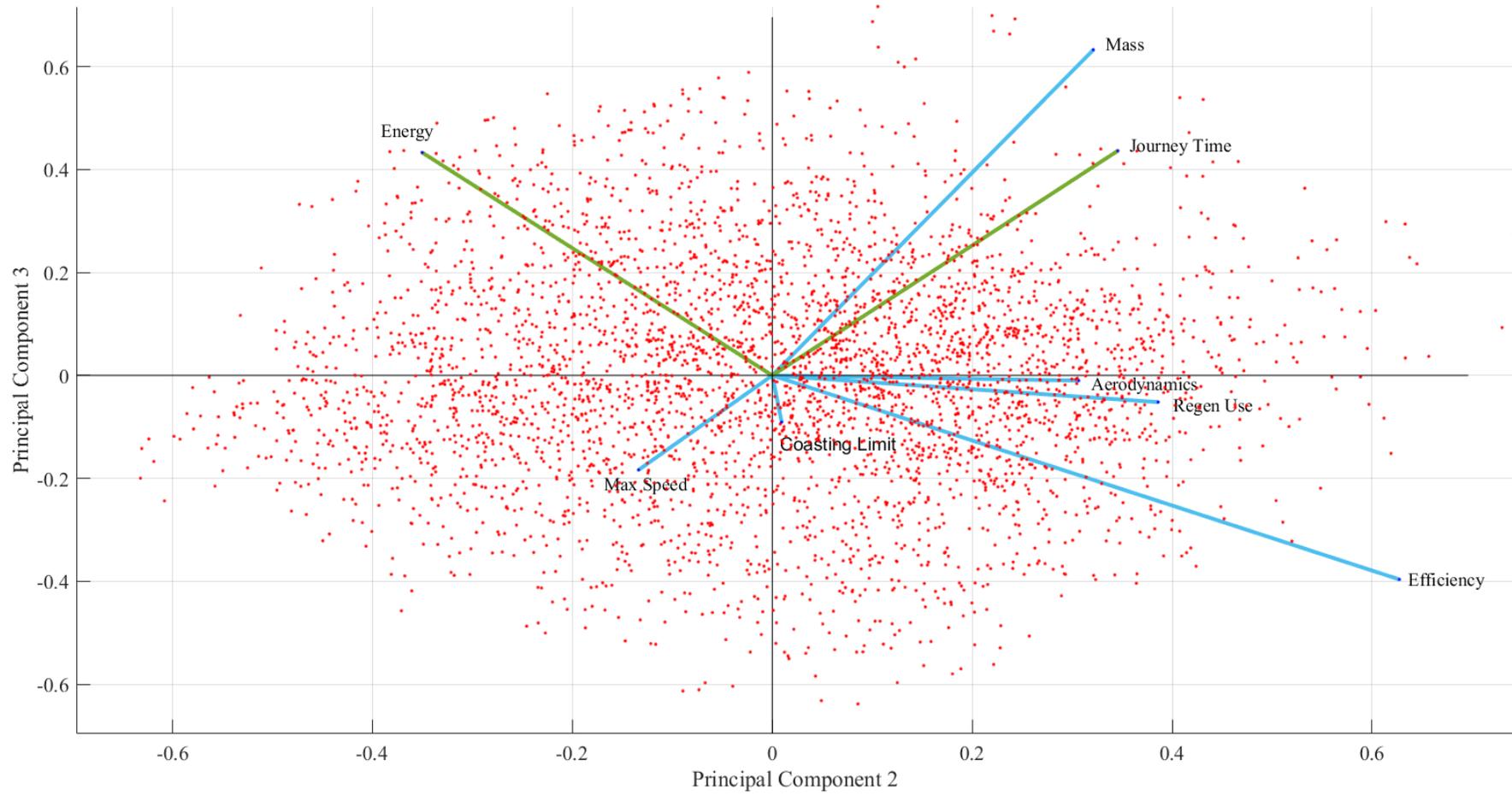
Figure 45: Bi-plot of PC2 and PC3 for ICHS subsystem with gradient of 10m/km

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6.3.5 High Speed Commuter (HSComm)

The importance rankings for the HSComm subsystem are extremely similar to those of the ICComm subsystem. The three critical factors for interstation distance in each instance are maximum speed, efficiency and coasting limit. However, in this case coasting is never the most important factor and drops in importance earlier within the distance range. The gradient results are also similar to the ICComm subsystem. Coasting limit and maximum speed have the most influence for steep downhill gradients, but significantly drop in importance as gradient increases. For steep uphill gradients, the efficiency, mass and maximum speed factors have the greatest impact on energy consumption.
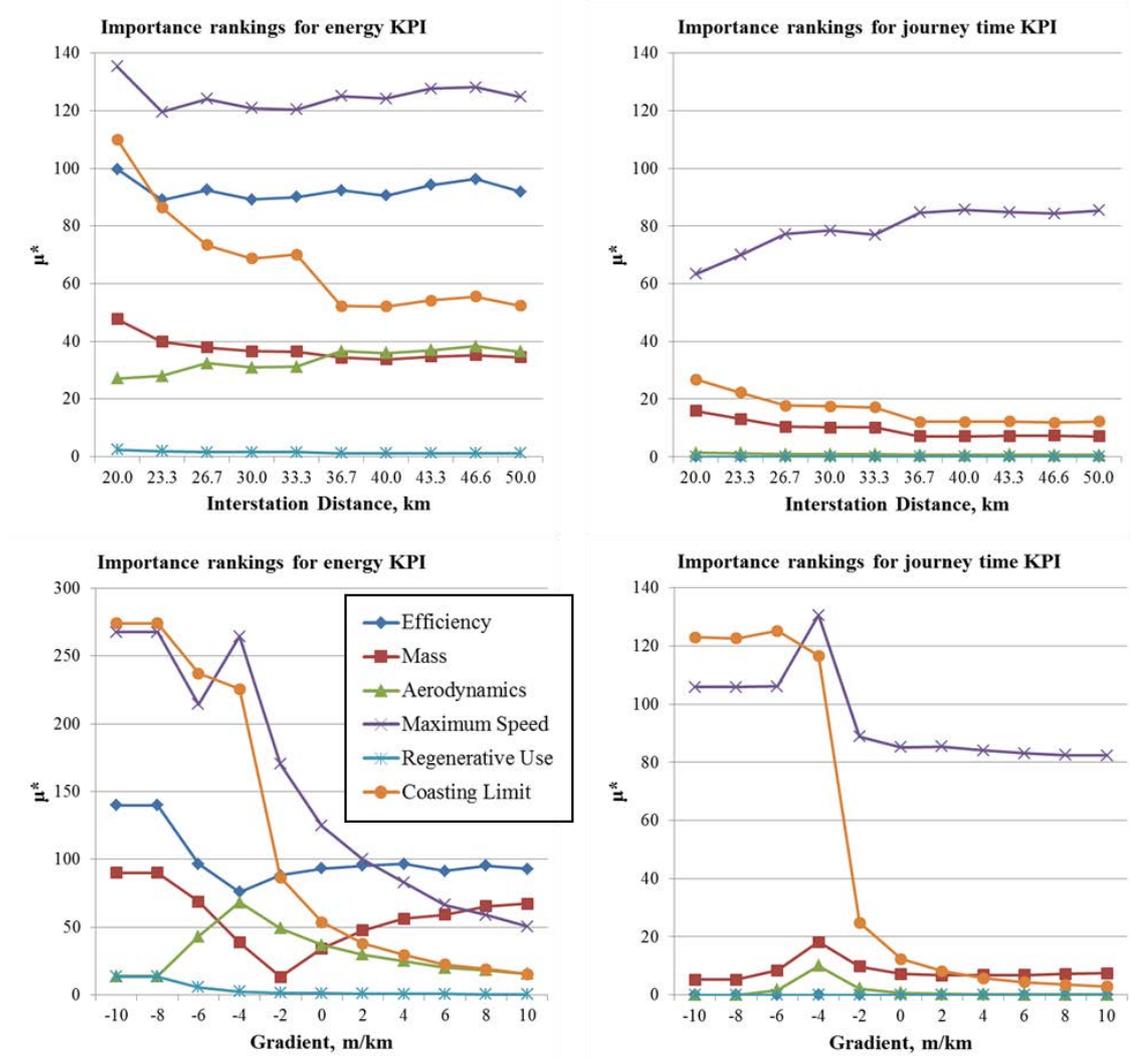
Figure 46: Importance rankings for all external factor values and KPIs for the HSComm subsystem

PCA analysis for the middle interstation distance (35 km) gave results that were almost identical to the ICComm maximum interstation distance results, indicating that the same conclusions can be drawn in this case. The gradient analysis also produced similar results and trends to the ICComm gradient analysis. The percentage contribution, PC scores and relevant TIP have been included in Appendix D for both analyses. The ICComm TIPs are shown alongside the interstation distance analysis to highlight the remarkable similarity in this particular case.

6.3.6 High Speed High Speed (HSHS)

The importance rankings for the High Speed High Speed subsystem show a distinct change from previous analyses, in that the coasting limit can no longer be considered as a key factor for either interstation distance or gradient. Efficiency and maximum speed are the only factors of real importance, and their rankings are opposite to those found previously, i.e., efficiency is ranked higher than maximum speed. If secondary factors were to be considered, then aerodynamics may have some influence. In terms of gradient, maximum speed has an influence on energy and journey time for downhill gradients but only efficiency is of significance for uphill gradients. Based on these results, the maximum interstation distance and maximum downhill and uphill gradients were chosen for PCA.
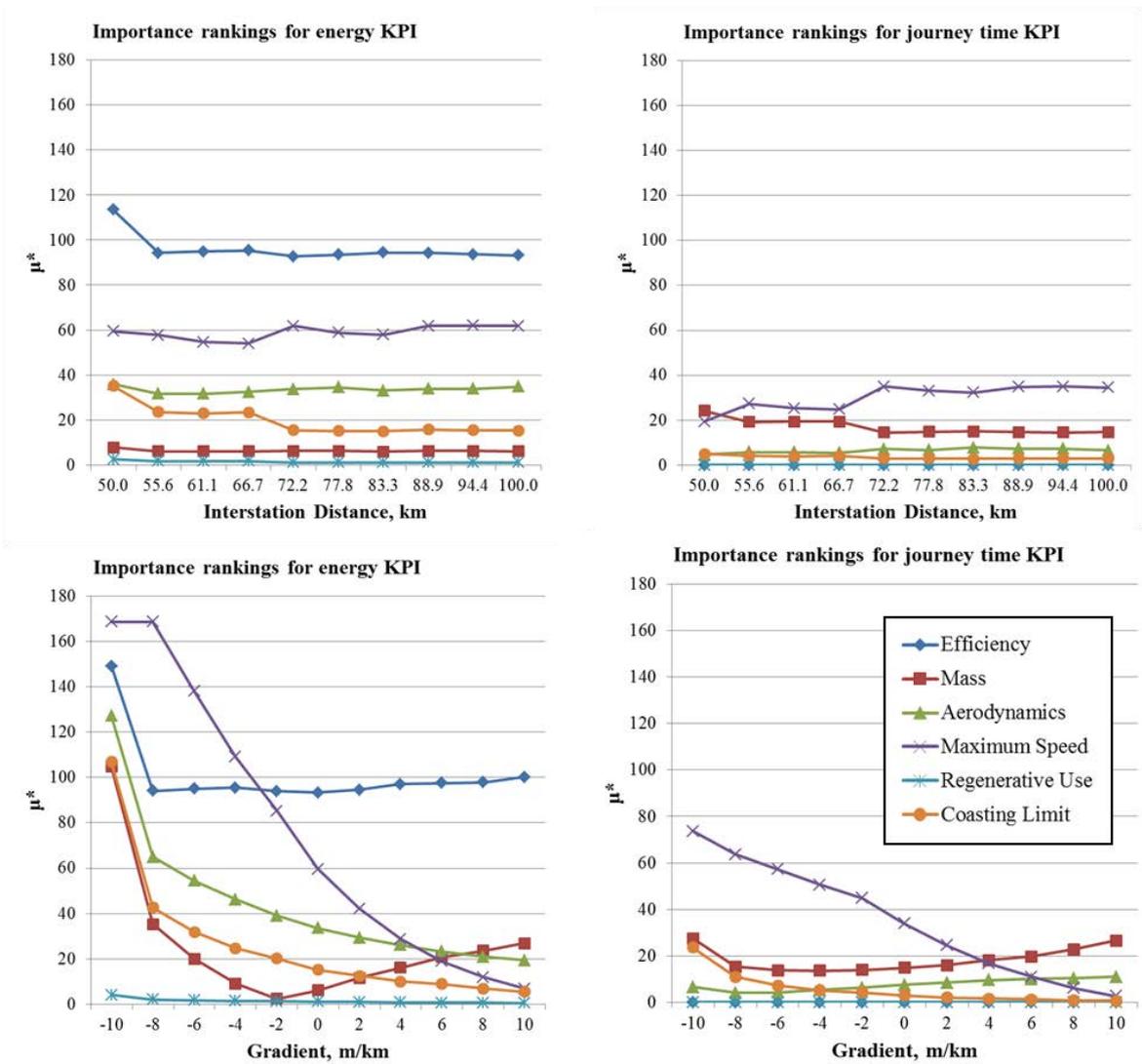
Figure 47: Importance rankings for all external factor values and KPIs for the HSHS subsystem

3.6.1 Analysis of interstation distance results

45% of the variation in the PCA is attributable to PC1, which again represents the trend between maximum speed, coasting limit, energy and journey time (Table 23). This makes sense as maximum speed is still the second most important factor. PCs 2 and 3 both point towards the increased importance of efficiency and aerodynamics. In each PC these two factors have significant PC scores and, although the energy and journey time values are not significant, they are higher than in the majority of previous analyses. This is represented in Figure 49, which is a bi-plot of PC2 and PC3.
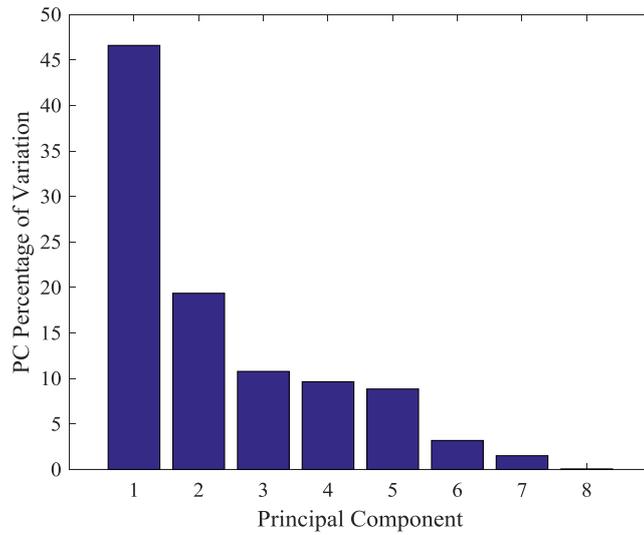
Figure 48: Percentage contribution of each PC to the total variation of the HSHS subsystem interstation distance dataset

Table 23: PC scores for HSHS subsystem with an interstation distance of 100 km

	PC1	PC2	PC3	PC4
Efficiency	-0.2	0.5	0.7	0.0
Mass	-0.2	0.5	-0.3	-0.7
Aerodynamics	-0.2	0.4	-0.5	0.1
Maximum Speed	-0.5	-0.1	0.1	0.0
Regeneration Use	-0.2	0.4	-0.1	0.7
Coasting Limit	-0.5	0.0	0.1	-0.1
Energy	-0.5	-0.3	-0.3	-0.1
Journey Time	0.5	0.3	-0.2	-0.1

The TIPs (Figure 50) for efficiency and maximum speed have very clear patterns showing their influence on energy, and energy and journey time respectively. However, contrary to previous analyses, aerodynamics does not display a linear trend with interactions, but instead loosely shows high values situated at the top of the curve and low values at the bottom. This was previously found to represent a local optimisation variable. The PCA implies a link between efficiency and aerodynamics which has some effect on energy and journey time, so this relationship was investigated. However, given the strength of the maximum speed correlation, only those dataset individuals with the minimum value of speed were used to generate Figure 51, which demonstrates an inverse relationship between the two factors.
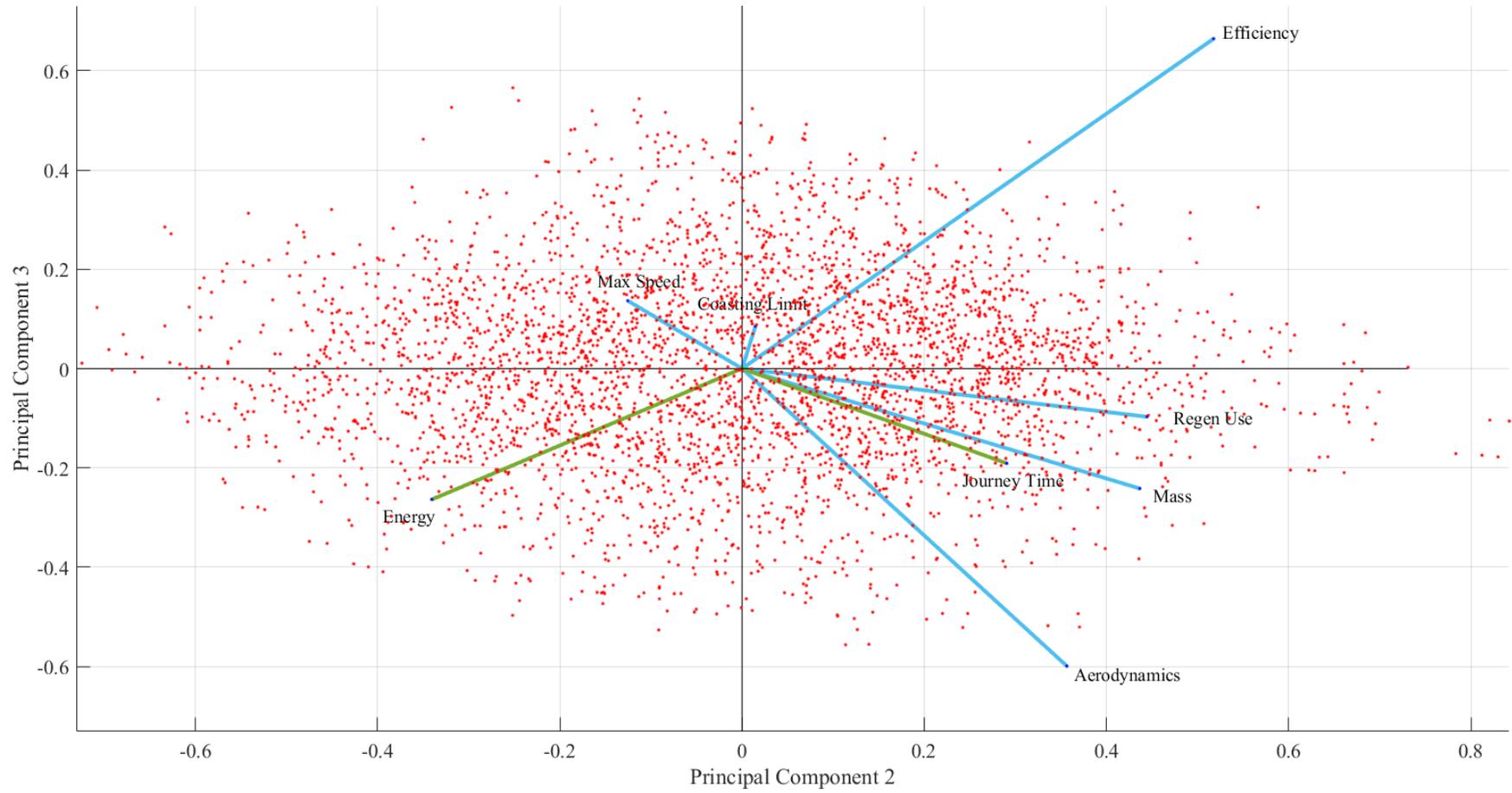
Figure 49: Bi-plot of PC2 and PC3 for HSHS subsystem with an interstation distance = 100 km
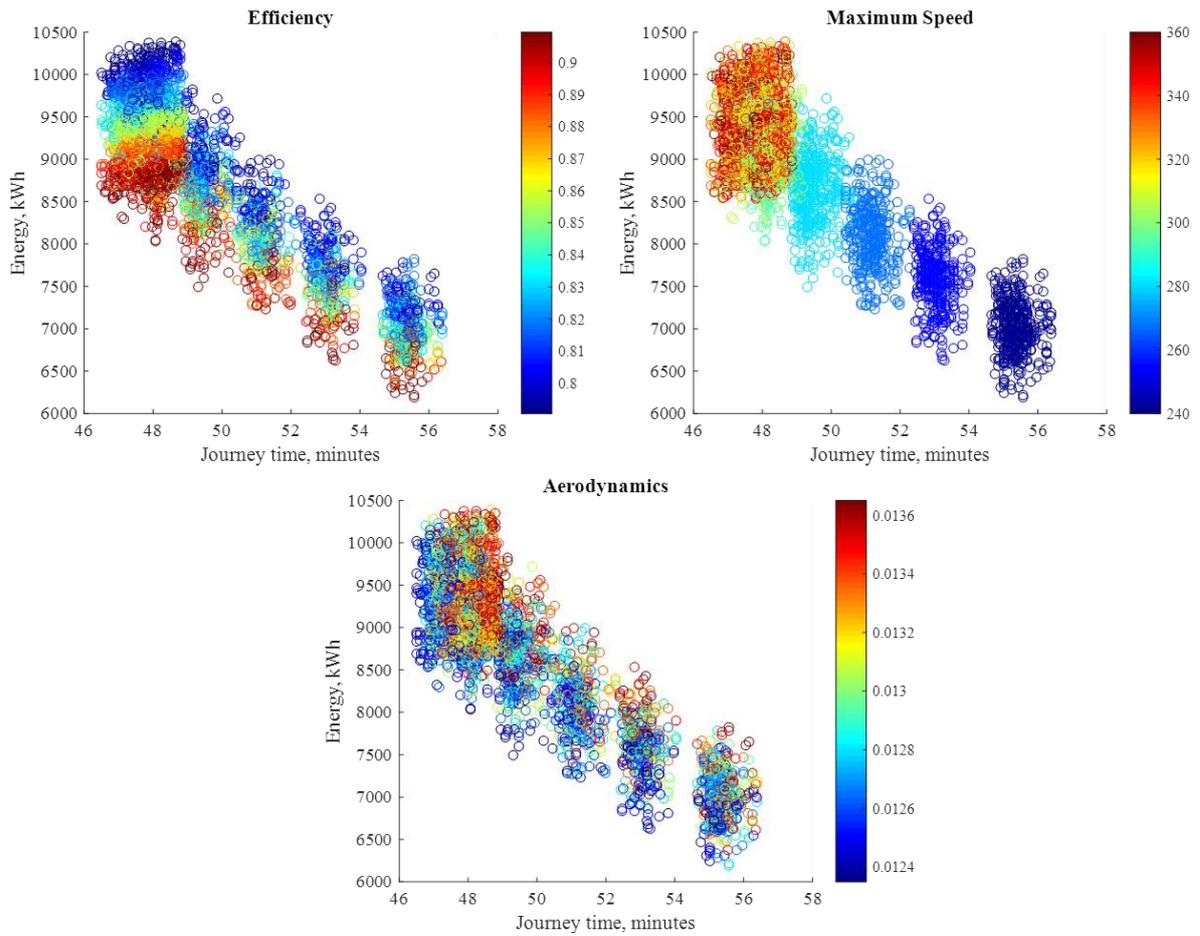
Figure 50: TIPs highlighting the relationships each of the three key factors have with energy and journey time, for the HSHS interstation distance dataset
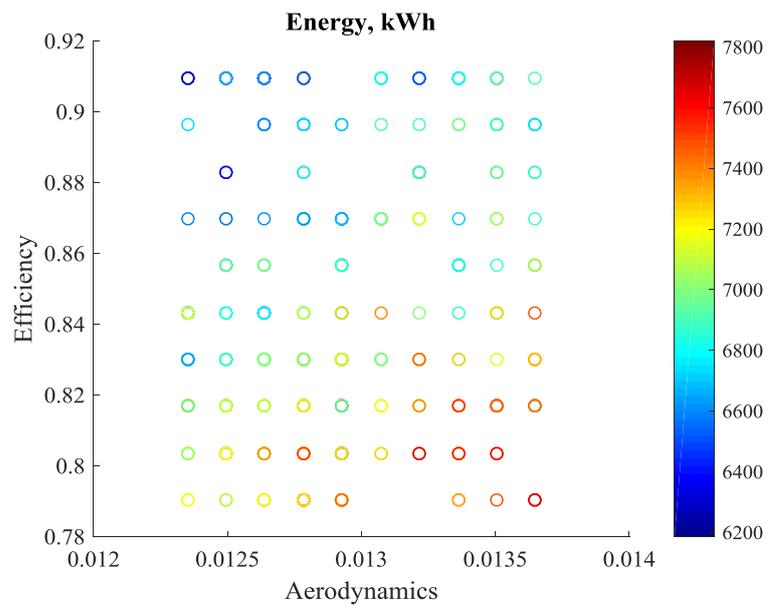
Figure 51: The correlation of energy with efficiency and aerodynamics for the HSHS maximum interstation distance individuals with maximum speed = 240 km/h

3.6.2 Analysis of gradient results

Maximum Downhill Gradient
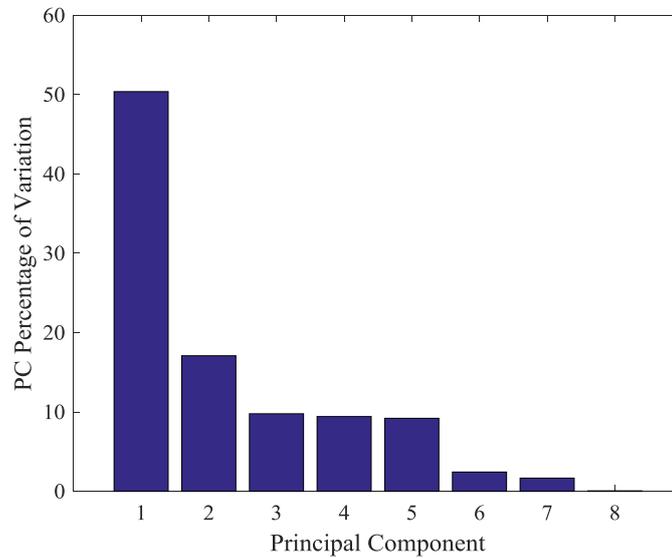
Figure 52: Percentage contribution of each PC to the total variation of the HSHS subsystem maximum downhill gradient dataset

Table 24: PC scores for HSHS subsystem with a gradient of -10 m/km

	PC1	PC2	PC3	PC4
Efficiency	-0.2	0.5	-0.1	0.7
Mass	-0.2	0.5	0.8	-0.1
Aerodynamics	-0.2	0.4	-0.6	0.0
Maximum Speed	-0.5	-0.2	0.1	0.0
Regeneration Use	-0.2	0.4	-0.2	-0.7
Coasting Limit	-0.5	-0.1	0.1	0.0
Energy	-0.5	-0.3	-0.1	-0.1
Journey Time	0.4	0.3	0.0	0.0

The percentage contribution of each PC is similar to the previous gradient analyses, and the first two PC scores are very close to the scores for the ICComm, HSComm and both Urban subsystems. Based on the PC scores and Morris rankings, the key factor which influences energy and journey time is maximum speed. PC2 indicates that efficiency, mass and aerodynamics also have a greater influence than in previous analyses. PCs 3 and 4 each point towards interactions between pairs of factors. However, these trends have little consequence in terms of energy or journey time. A bi-plot of PCs 1 and 2 is shown in Figure 53.
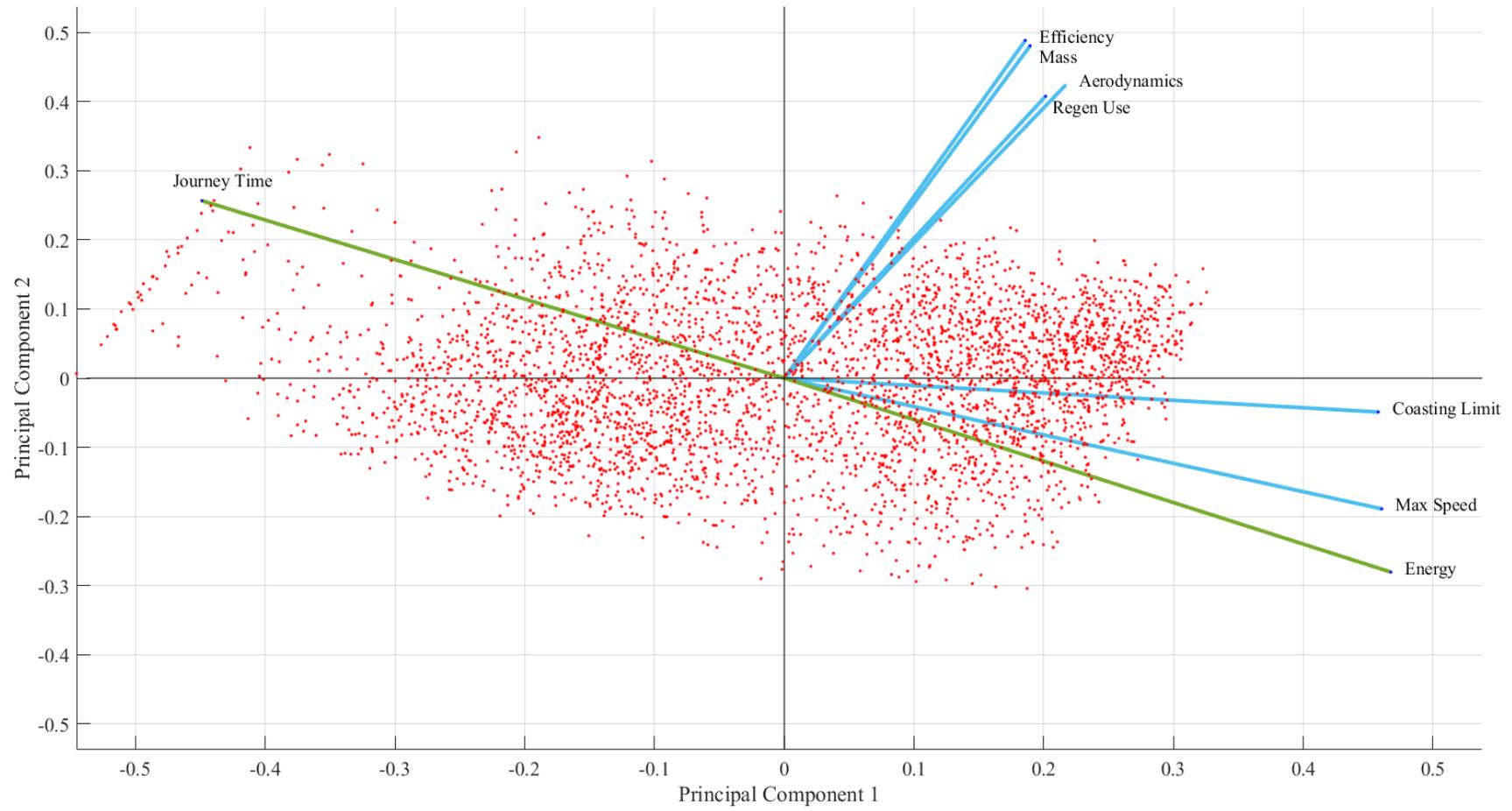
Figure 53: Bi-plot of PC1 and PC2 for HSHS subsystem dataset with a gradient of -10m/km

The TIPs for the maximum downhill gradient (Figure 54) indicate strong relationships between energy, journey time and maximum speed and efficiency, and once again aerodynamics presents as a local optimisation variable. The coasting limit shows some influence for energy and journey time, which corresponds with the Morris SA. However, unlike previous analyses, the trend for mass is unclear.
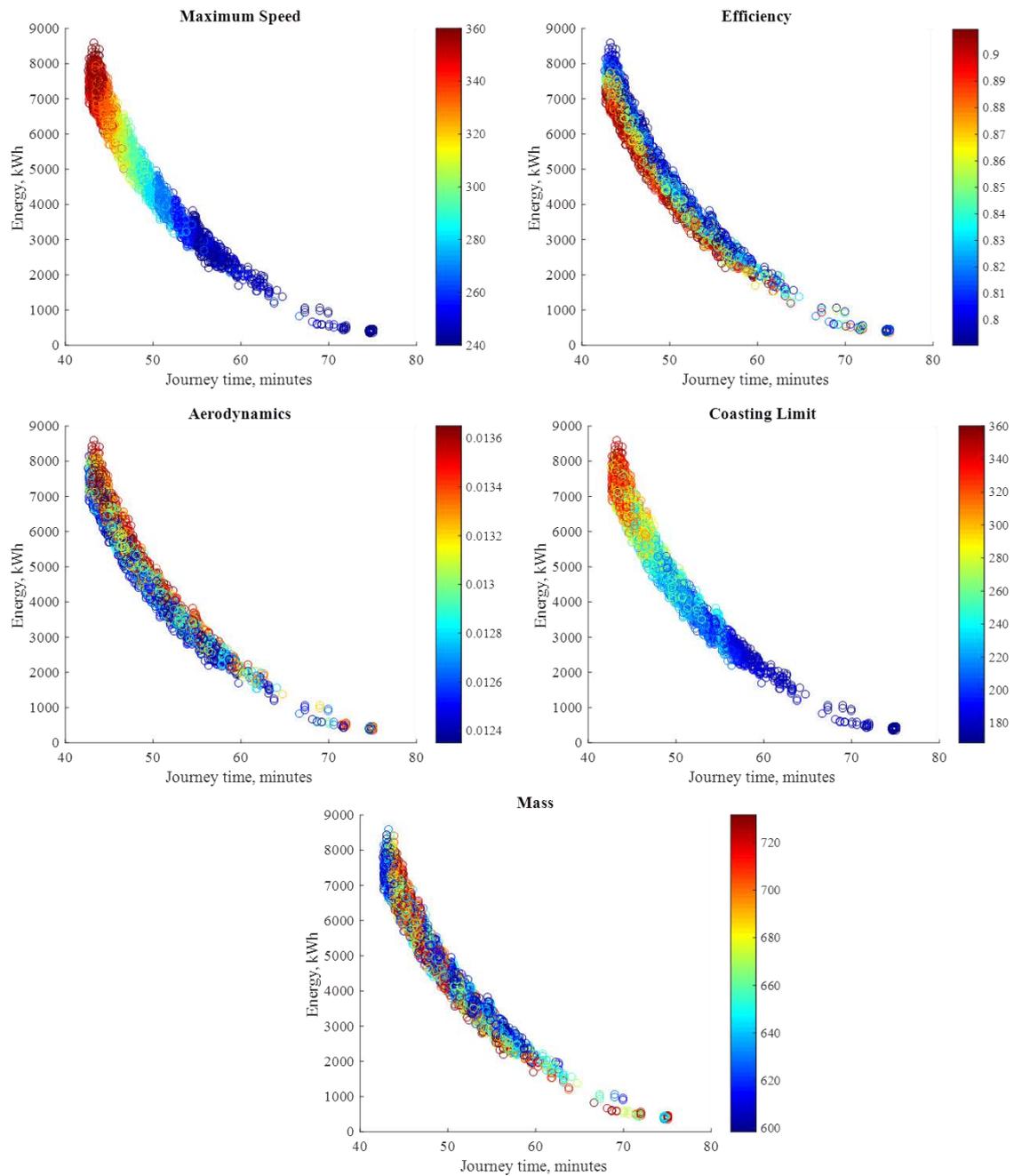
Figure 54: TIPs highlighting the relationships each of the top five factors have with energy and journey time, for the HSHS maximum downhill gradient dataset

Although PC3 indicates a relationship between mass and aerodynamics, as this PC has no relationship with energy and journey time it is unlikely that mass and aerodynamics alone would show correlation on a TIP. However, PC2 does have some influence on energy and journey time and indicates a relationship between mass, aerodynamics and efficiency. As with the interstation distance analysis, a group of individuals with the same maximum speed were isolated to evaluate the relationship between two factors without interference from the strong speed trend. In this instance, the highest maximum speed was chosen. Figure 55 confirms the existence of a relationship between the three variables, which would account for the lack of clarity in the mass TIP.
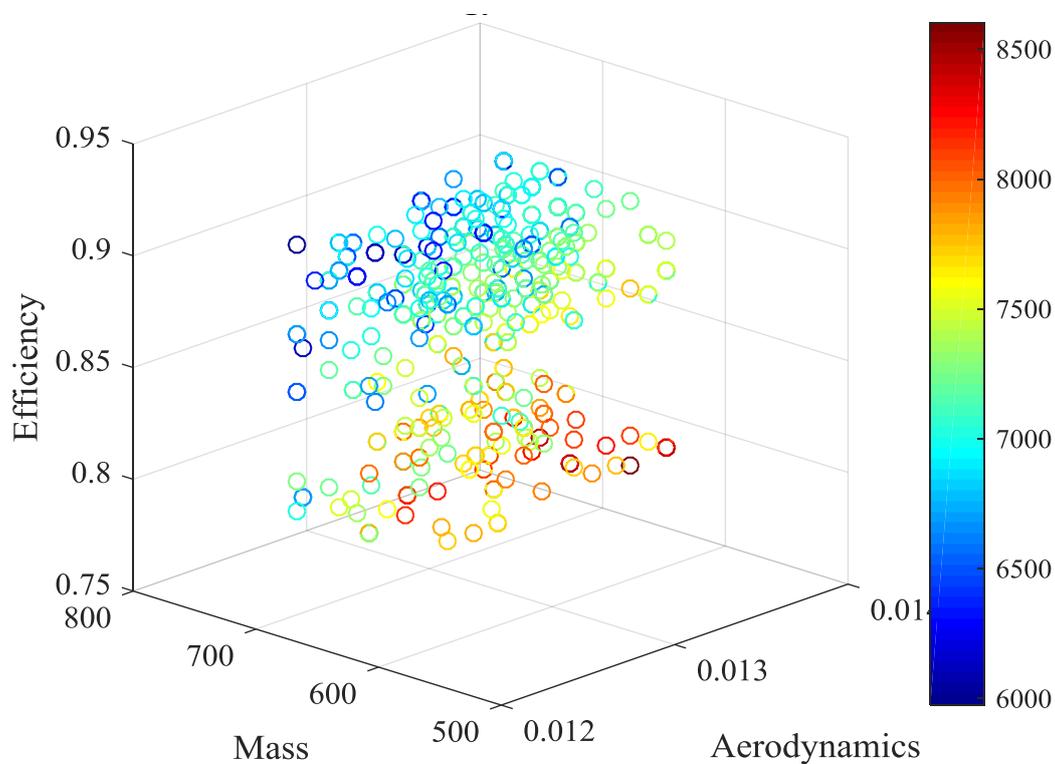
Figure 55: The correlation of energy with efficiency, aerodynamics and mass for the HSHS maximum downhill gradient individuals with maximum speed = 360 km/h

Maximum Uphill Gradient
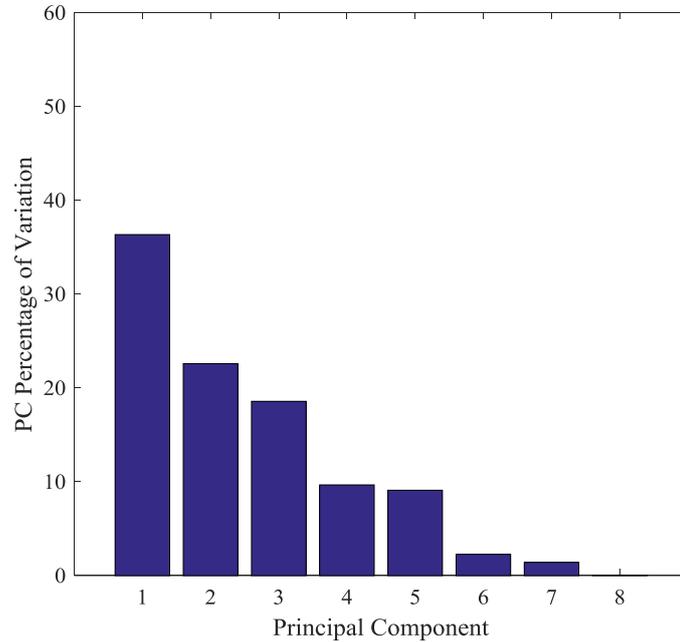
Figure 56: Percentage contribution of each PC to the total variation of the HSHS subsystem maximum uphill gradient dataset

Table 25: PC scores for HSHS subsystem with a gradient of 10 m/km

	PC1	PC2	PC3	PC4
Efficiency	0.4	-0.6	-0.1	0.2
Mass	0.4	0.2	0.5	0.3
Aerodynamics	0.3	0.0	0.0	-0.9
Maximum Speed	0.4	0.3	-0.5	0.2
Regeneration Use	0.3	0.1	-0.1	-0.2
Coasting Limit	0.4	0.2	-0.4	0.2
Energy	-0.1	0.7	0.1	-0.1
Journey Time	0.4	0.0	0.6	0.1

The percentage contributions of each PC and the PC scores have changed significantly from previous analyses (Figure 56). The first PC, which accounts for just over 35% of the variation in the dataset, indicates a positive correlation between mass, maximum speed, coasting limit and journey time (efficiency cannot influence journey time due to the simulator programming). However, PC3 also shows a relationship which affects journey time, but in this case a high mass value but low values of maximum speed and coasting limit increase journey time. From this it can be deduced that mass is the only factor that influences journey time, which corroborates the Morris results. Both PCs are plotted in Figure 57.

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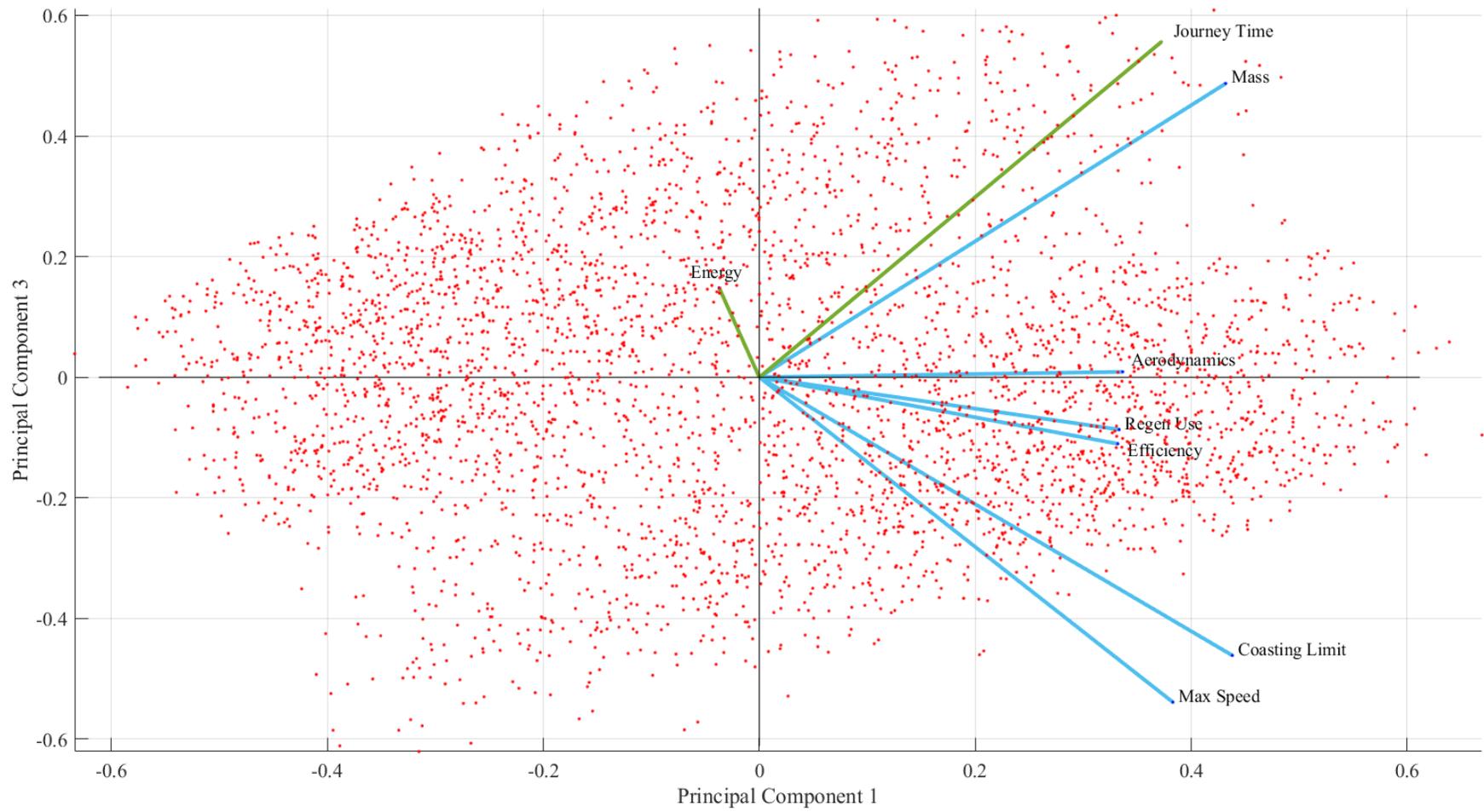
Figure 57: Bi-plot of PC1 and PC3 for HSHS subsystem dataset with a gradient of 10 m/km
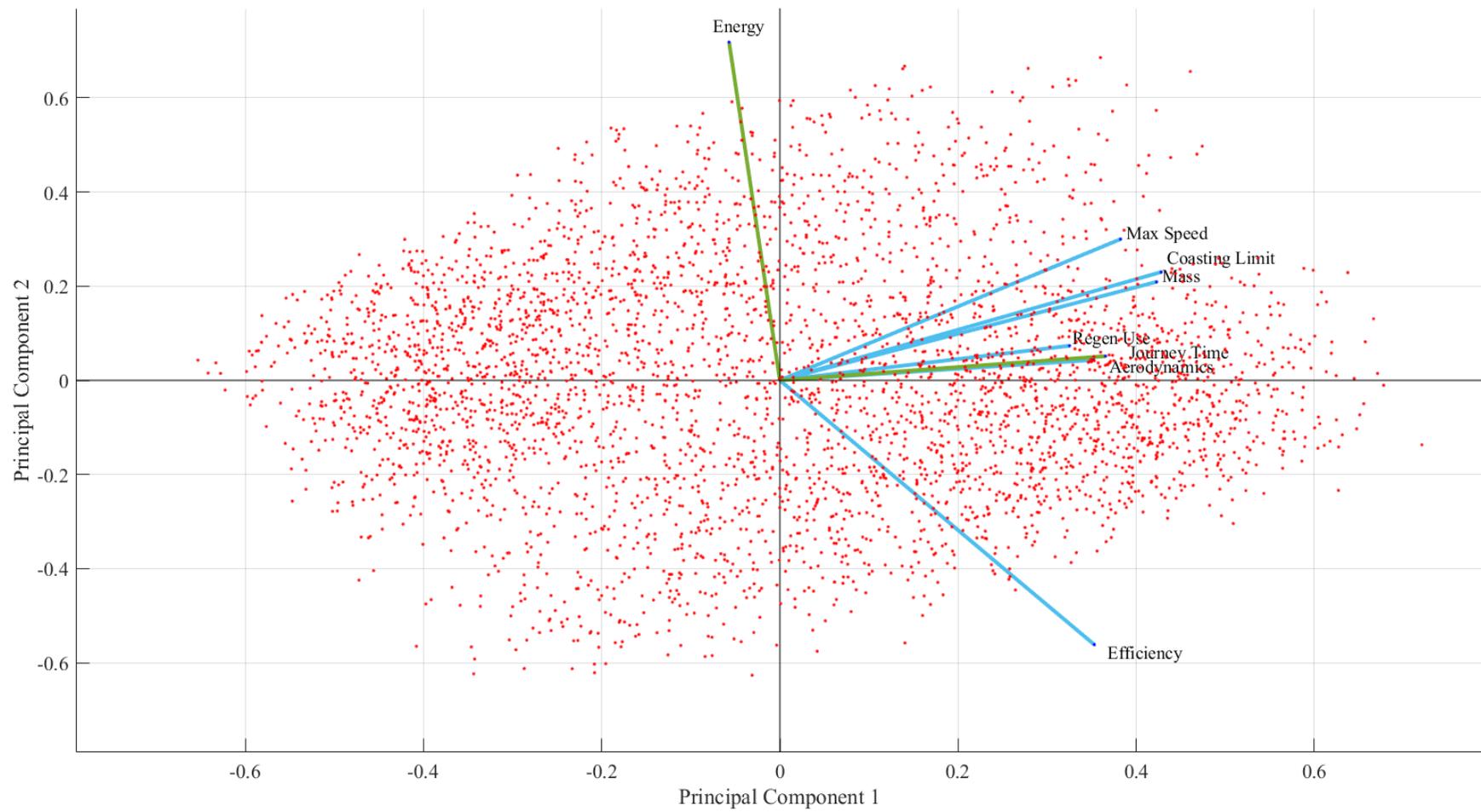
Figure 58: Bi-plot of PC1 and PC2 for HSHS subsystem dataset with a gradient of 10 m/km

PC2 indicates that efficiency is the sole factor affecting energy, which is illustrated in Figure 58. Both of these strong relationships are confirmed by the TIPs in Figure 59 which have extremely clear colour graduation against energy (y-axis) for efficienc, and journey time (x-axis) for mass.
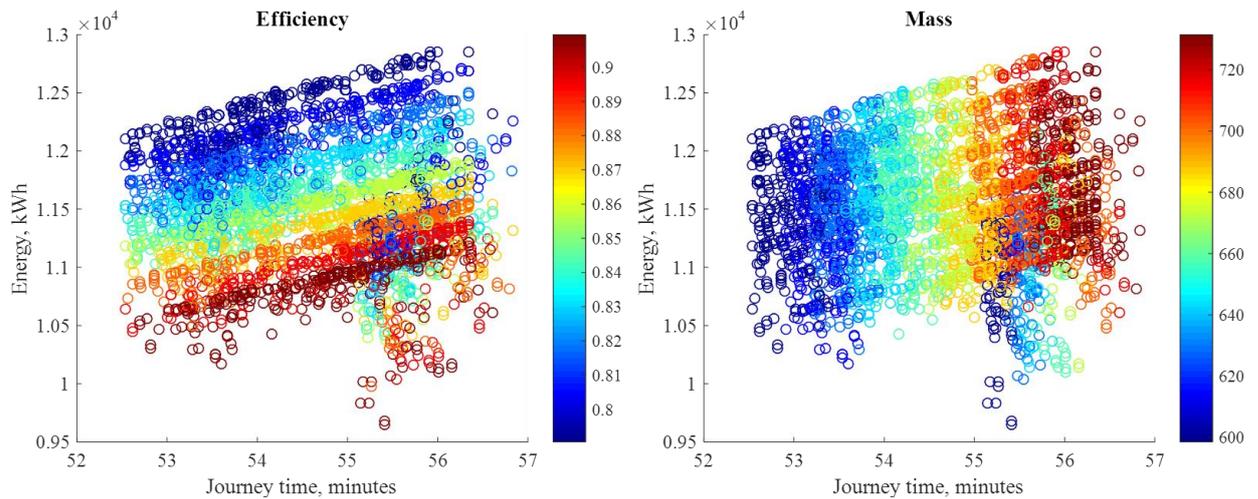
Figure 59: TIPs highlighting the relationships between efficiency and energy, and mass and journey time, for the HSHS maximum uphill gradient dataset

6.4 Stage 7: System Results

In Section 3, the Morris results for each subsystem were presented individually, and PCA analyses conducted on points of interest regarding the effect of interstation distance or gradient. In order to understand the overall system, the data is considered in three different ways:

- Firstly, the results are summarised in tabular form, allowing initial conclusions to be drawn as to the relationships between subsystems and factors. Tables 26 and 28 give the key and secondary factors influencing energy and journey time for each of the six subsystems and detail the effect of increasing the interstation distance and gradient respectively. Tables 27 and 29 summarise the relationships between the factors and energy for each subsystem. Next, the relationships between subsystems are explored using heat map visualisations for interstation distance and gradient. In order to do this, at each point of interstation distance or gradient, the 6 $\mu*$ values for the factor set are encoded into one unique number.

- Secondly, the relationships between the internal factors, external factors and subsystems are investigated using height maps, and the trends summarised using area charts.

The relationship between the internal factors and journey time is not considered between subsystems. The Morris results agree for all subsystems that the key factors influencing journey time are maximum speed and coasting limit and the secondary factor is mass. The influence of the coasting limit on journey time correlates with its importance ranking for energy.

6.4.1 Tabulated Results

The tabulated results (Tables 26-29) were intended to simplify the important factors and trends for each subsystem, allowing basic deductions to be made about the relationships between the subsystems and factors.

For Tables 26 and 28, the dominant factors were defined as the three that exhibit the highest $\mu*$ values. The secondary factors were then the next two highly ranked factors. However, when there was a large gap between factor $\mu*$ values (as for UU and HSHS subsystems) only the two highest factors were defined as dominant. Equally, when the $\mu*$ values of the secondary factors were very low, they were discounted.

Tables 27 and 29 summarise the key trends, as described based on the TIPs for each subsystem. 'Linear' describes a TIP that shows correlation between the factor and the KPIs. The difference between 'Strong Linear' and 'Linear' was determined by the distinctness of the colour graduation on the plot, although being visual, this was subjective. 'Local' refers to those factors which were found to act as local optimisation variables when investigated further, e.g., mass for UU subsystems.

Accepting the subjective nature of such distinctions, the following observations were made:

- The solutions for an Urban network are the same regardless of the service;

- Commuter services on both Inter-city and High Speed networks display the same importance rankings, despite the network differences;

- Maximum speed and efficiency are always key or secondary factors;

- High Speed services are better candidates for aerodynamic improvement;

- Commuter services and Urban subsystems are better candidates for mass improvement;

- The influence of coasting decreases as the interstation distance increases;

- Maximum speed and coasting limit are directly related to the energy and journey time results of a subsystem;

- Mass and efficiency generally have a secondary relationship with the KPIs, acting as local optimisation variables. The exception is the HSHS subsystem.

Table 26: The key and secondary factors for each subsystem based on the interstation distance results

Network	Service	Initial Order (Minimum Interstation Distance)		Effect of Interstation Distance	Order at Maximum Interstation Distance
		Dominant Factors	Secondary Factors		
Urban	Urban	Coasting Limit	Efficiency	None	No Change
		Maximum Speed	Mass		
Urban	Commuter	Same as above			
Inter-city	Commuter	Coasting Limit	Aerodynamics	Decreasing Importance of Coasting Limit	Maximum Speed
		Maximum Speed	Mass		Efficiency
		Efficiency			Coasting Limit
Inter-city	High Speed	Maximum Speed	Aerodynamics	Decreasing Importance of Coasting Limit	Maximum Speed
		Efficiency			Efficiency
		Coasting Limit			Aerodynamics
High Speed	Commuter	Maximum Speed	Aerodynamics	Decreasing Importance of Coasting Limit	Maximum Speed
		Coasting Limit	Mass		Efficiency
		Efficiency			Coasting Limit
High Speed	High Speed	Efficiency	Aerodynamics	None	No Change
		Maximum Speed			

Table 27: The relationships displayed by each factor for the interstation distance analyses

	UU	UComm	ICComm (min)	ICComm (max)	ICHS	HSComm	HSHS
Coasting Limit	Strong Linear	Strong Linear	Strong Linear	Linear	Linear	Linear	
Maximum Speed	Linear	Linear	Linear, Interaction with Coasting Limit	Strong Linear	Strong Linear	Strong Linear	Strong Linear
Efficiency	Local	Local	Interaction between Coasting Limit, Mass and Efficiency	Local	Local	Local	Local
Mass	Local	Local		Local		Local	
Aerodynamics				Interactions	Interactions	Interactions	Weak Local, Interaction with Efficiency

Table 28: The key and secondary factors for each subsystem based on the gradient results

Network	Service	Initial Order (Maximum Downhill Gradient)		Effect of Gradient	Order at Maximum Uphill Gradient
		Dominant Factors	**Secondary Factors**		
Urban	**Urban**	Coasting Limit	Efficiency	Decreased Importance of Key Factors	Efficiency
		Maximum Speed	Mass		Coasting Limit
					Maximum Speed
Urban	**Commuter**	Same as above			
Inter-city	**Commuter**	Coasting Limit	Efficiency	Decreased Importance of Key Factors	Efficiency
		Maximum Speed	Mass		Mass
					Maximum Speed
Inter-city	**High Speed**	Coasting Limit	Efficiency	Decreased Importance of Key Factors	Efficiency
		Maximum Speed	Mass		Mass
			Aerodynamics		Maximum Speed
High Speed	**Commuter**	Coasting Limit	Efficiency	Decreased Importance of Key Factors	Efficiency
		Maximum Speed	Mass		Mass
					Maximum Speed
High Speed	**High Speed**	Maximum Speed	Aerodynamics	Decreased Importance of Key Factors	Efficiency
		Efficiency	Mass		Mass

Table 29: The relationships displayed by each factor for the gradient analyses

	UU	UComm	ICComm	ICHS	HSComm	HSHS (down)	HSHS (up)
Coasting Limit	Strong Linear	Strong Linear	Linear	Weak Linear	Linear	Linear	
Maximum Speed	Linear	Linear	Strong Linear	Linear	Strong Linear	Strong Linear	
Efficiency	Local, Interaction	Local, Interaction	Strong Local	Strong Local	Strong Local	Strong Local	Linear (energy)
Mass	Local	Local	Strong Local	Strong Local	Strong Local	Interaction with Aerodynamics and Efficiency	Linear (journey time)
Aerodynamics				Interactions		Local	

6.4.2 Heat Map Visualisation

Heat maps were generated for both interstation distance (Figure 61) and gradient (Figure 62) by encoding the $\mu*$ results for the energy KPI so that each distinct set of rankings equated to a unique number, which could then be used to colour the heat maps. Figure 60 shows the $\mu*$ results for the Inter-city High Speed subsystem with two different sets of rankings highlighted.
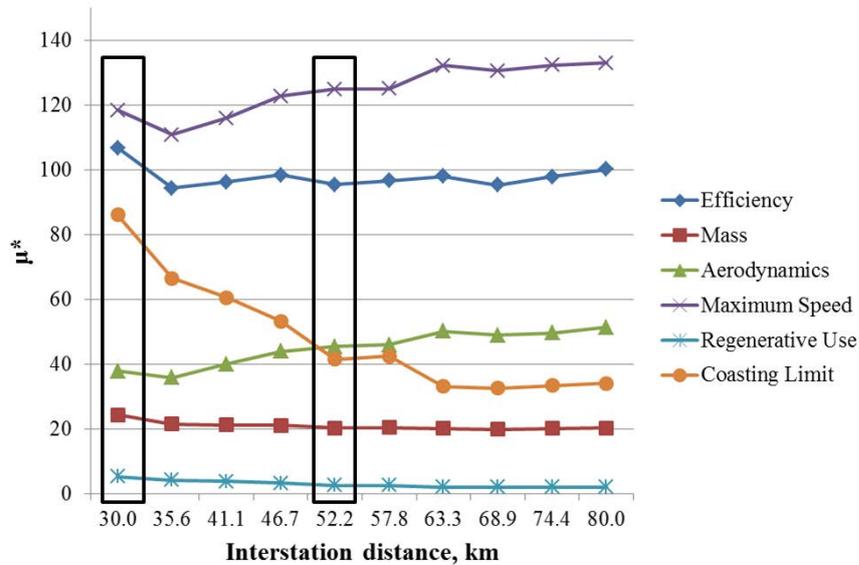
Figure 60: Two distinct sets of rankings indicated on the ICHS subsystem μ* results for the energy KPI

For each set of rankings, every factor was equated to a prime number which was then multiplied by a simple number based on the factor ranking. The sum of these calculations gave the unique number for the set. To ensure that each combination is truly unique, there must be no overlap between the multiplier sets. Table 30 details the prime numbers and multipliers used. Table 31 shows the calculations for the two ICHS ranking sets above.

Table 30: The equivalent factor numbers and ranking multipliers used to generate unique numbers

Factor	Prime Number	Ranking Order	Simple Multiplier
Efficiency	7	1st	6
Mass	11	2nd	5
Aerodynamics	13	3rd	4
Maximum Speed	17	4th	3
Regenerative Use	19	5th	2
Coasting Limit	23	6th	1

Table 31: Example calculations of unique numbers, using the two distinct ranking sets from Figure 59

Factor	Prime Number	Rank Set 1	Simple Multiplier	Product	Rank Set 2	Simple Multiplier	Product
Efficiency	7	2nd	5	35	2nd	5	35
Mass	11	5th	2	22	5th	2	22
Aerodynamics	13	4th	3	39	3rd	4	52
Maximum Speed	17	1st	6	102	1st	6	102
Regenerative Use	19	6th	1	19	6th	1	19
Coasting Limit	23	3rd	4	92	4th	3	69
Unique Number				**309**			**299**
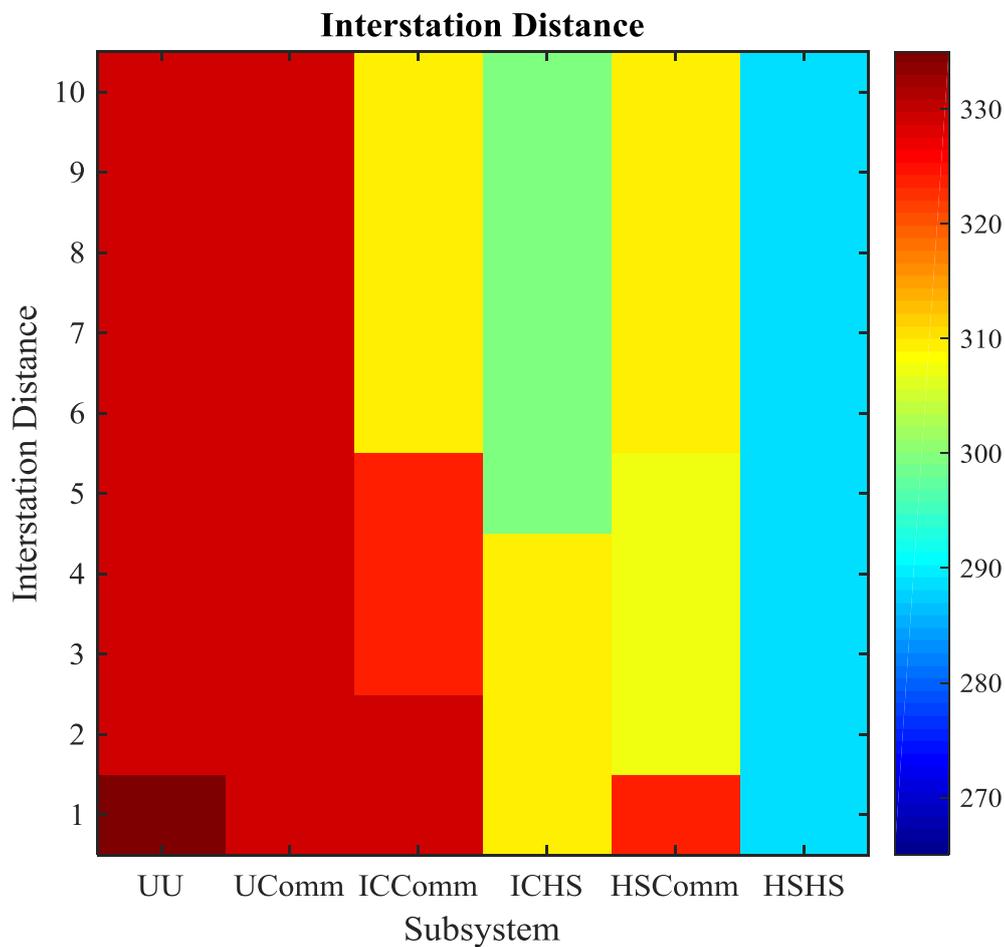
Figure 61: Heat map visualisation of interstation distance µ* results for all subsystems

The heat map in Figure 61 gives greater detail about the relationships between subsystems and interstation distance, which can be used to build upon the previously made simple deductions from the tabular results. Generally speaking, the higher the value, the greater is the importance of the coasting limit, as this has the highest prime multiplier. Whereas the lower

the value, the greater is the importance of efficiency which has the lowest multiplier, The colouring above indicates three distinct groups of subsystems:

- The 'red' group containing the services running on Urban networks, group 1

- The 'blue' group containing solely the HSHS subsystem, group 2

- The 'orange' group which contains the remaining three subsystems, group 3

Considering each group in more detail, it can be seen that the interstation distance has a minimal impact on group 1 and no influence on group 2. This means that the solutions for these groups are independent of their service stopping patterns. Group 3 has a variation in colouring along both axes, indicating that interstation distance has an impact and also that some fundamental differences exist between the group's subsystems. For each subsystem, significant changes due to interstation distance occur around the median interstation distance value for that subsystem. As expected out of these subsystems the two Commuter services are closest, although some differences do exist. These are likely caused by the differences in the importance of the coasting limit, which drops much sooner (relative to the interstation distance increases) for HSComm services. However, it is interesting to note that ICHS services with a shorter interstation distance require the same solutions as Commuter services with a longer interstation distance.

The same three groups are identifiable on the gradient heat map in Figure 62. In group 1, the solutions are largely the same as for interstation distance, and only begin to change for steep uphill gradients. In group 2 the solutions are the same as for interstation distance only around the midpoint (-2 to 2 m/km). Before and after this point the solutions differ depending on whether the gradient is up or downhill. These points of change are also evident in group 3, and have significant colour changes. However, there are a lot more subtle changes within these distinctive regions than for the other groups. Another way to consider this heat map is in three loosely diagonal groups based on colour: red (bottom left), blue (top right) and green (middle diagonal).
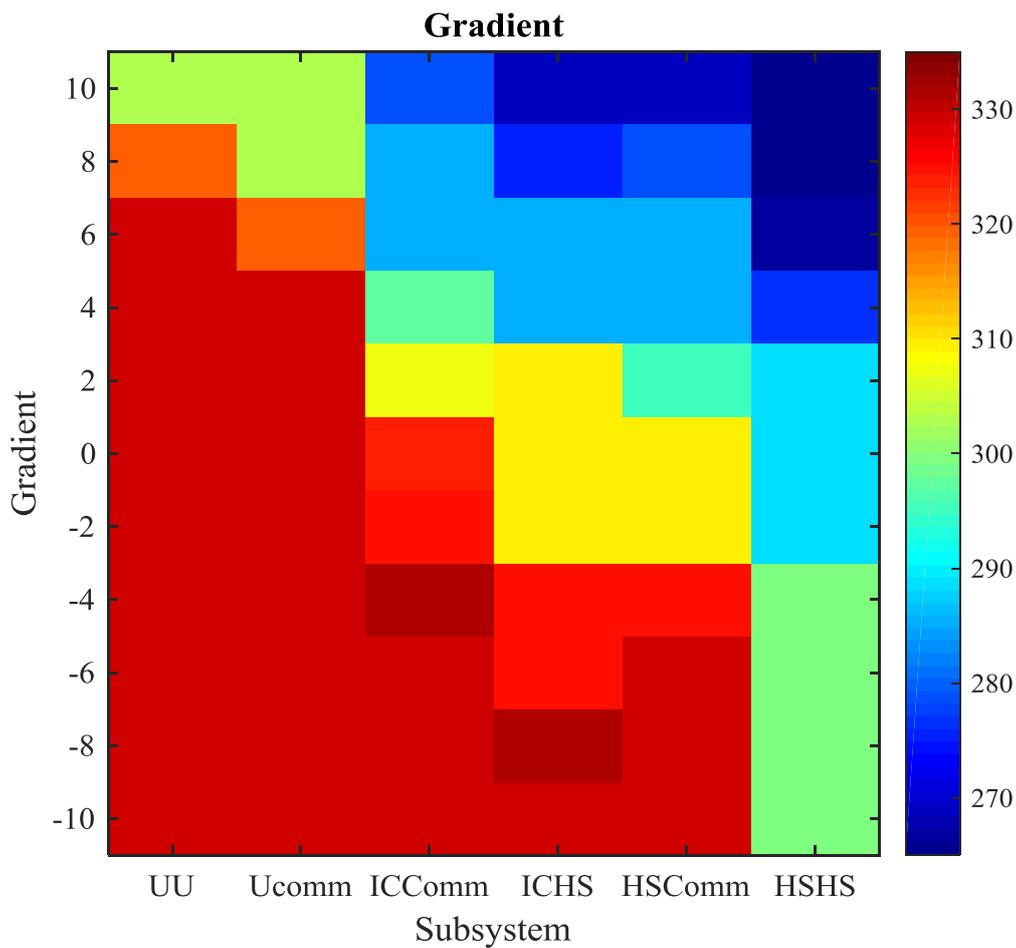
Figure 62: Heat map visualisation of gradient μ* results for all subsystems

6.4.3 Height Map Visualisation

Based on the Morris results for each subsystem and the tabular summary, it can be inferred that the significant colour differences in the heat maps are due to the coasting limit variable, and that subtle changes are caused by changes in less important factors, such as aerodynamics and mass. However, in order to understand these relationships better, height maps have been generated that show the change in μ* for each internal factor based on both the external factor value and subsystem. Regeneration use is not included in the analysis because it was never previously classified as a key or secondary factor. Note the $\mu*$ value is used for colour as well as height.

Note that, although the height maps and subsequent area charts are shown as continuous between subsystems, that the values for each subsystem are discrete, meaning that the graphs cannot be used to interpolate values between the subsystems.

Interstation Distance
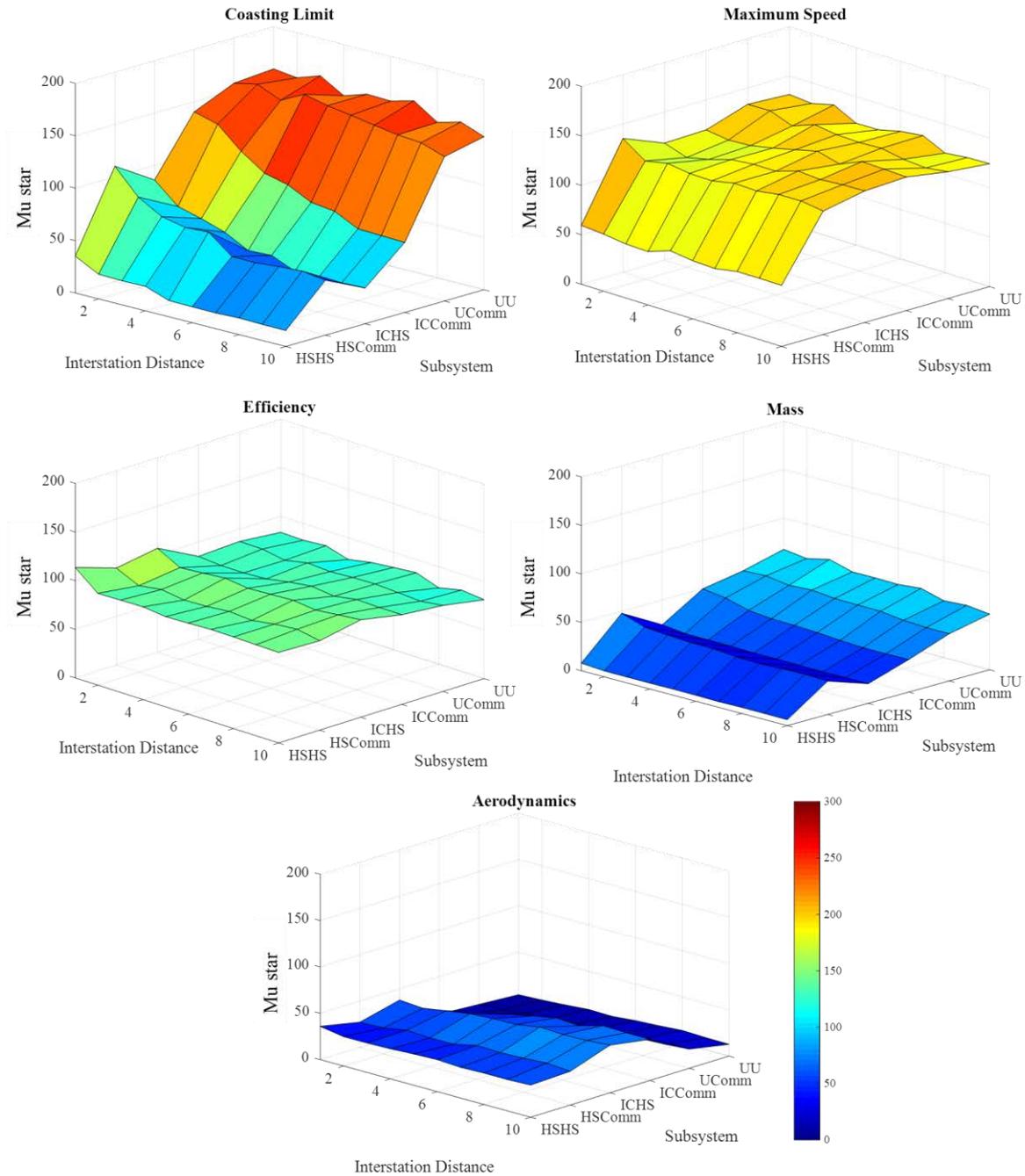
Figure 63: Height maps of μ* value against interstation distance for each subsystem

Once again for interstation distance, 1 represents the shortest interstation distance and 10 the largest. If the coasting limit plot is excluded, the height maps in Figure 63 generally show very little variation in colour for each subsystem along the bottom left axis, indicating that interstation distance has minimal impact on the μ^* values. The exception to this is the importance of coasting limit for HSComm and ICComm services, which increases for shorter

interstation distances. Working from the least to the most important factors, the differences between subsystems are as follows:

- Aerodynamics has minimal variation in $\mu*$ based on subsystem, and peaks for Inter-city services;

- Mass displays a general decline in importance as the subsystem changes from Urban through to High Speed, with a surge for HSComm services;

- Mass and aerodynamics interchange in terms of importance depending on the subsystem, but always remain the two least important factors;

- The efficiency plot is fundamentally level over the entire range of subsystems indicating that is equally important in all cases. However, its ranking does change depending on the $\mu*$ values of maximum speed and coasting limit;

- The maximum speed remains the second most important factor for all subsystems excluding HSHS. At this point, there is a significant drop in importance which brings it below efficiency;

- The coasting limit exhibits the most variation out of the internal factors. As well as significantly dropping in importance as the subsystems change from Urban through to High Speed, the severity of decline depends on the interstation distance. Although noteworthy, the change in μ* is less for smaller interstation distances.

Because the interstation distance generally has a minimal impact on factor importance, the key trends for the different factors and subsystems can be summarised using an area plot, as shown in Figure 64. The average of the $\mu*$ interstation distance values are plotted for each subsystem and factor.
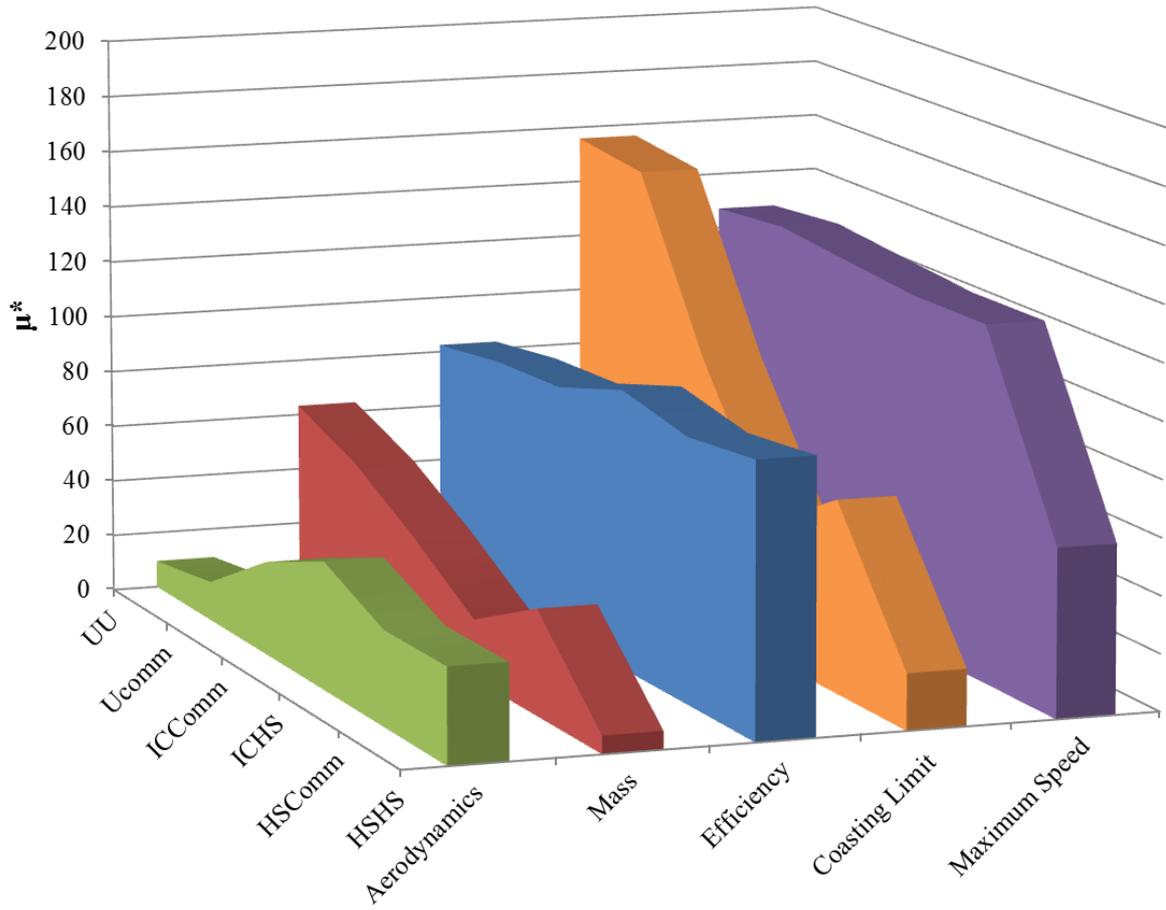
Figure 64: Area plot showing the key trends for the energy KPI based on the μ* interstation distance values

Gradient
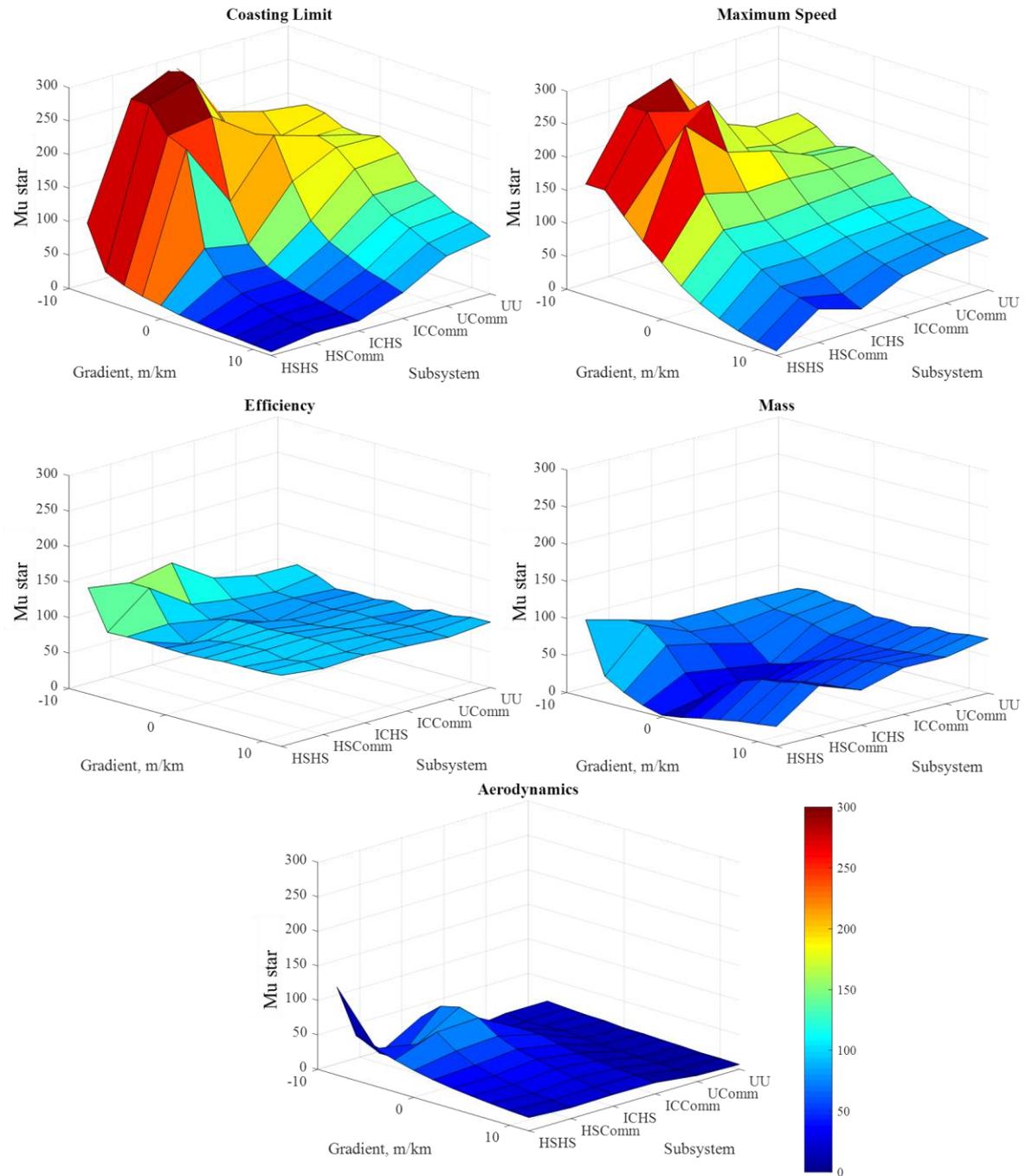
Figure 65: Height map of μ* value against gradient for each subsystem

The gradient height maps (Figure 65) show that both the subsystem and the value of the gradient have an impact on the importance of factors. Generally speaking, the μ* values for factors are higher in the bottom left corner of the graphs than on any other part of the plot, i.e.,

for steep downhill gradients on High Speed lines or services. However, these increases are not in proportion between the subsystems or factors so the rankings do change. Working from the least to the most important factors, the differences in terms of gradient and subsystem are as follows:

- The importance of aerodynamics effectively remains low and level across subsystems and gradient values. The exception is for High Speed services where, as the gradient drops below zero, the importance increases.

- Based on the colour of the plot, the importance of mass also generally remains level. As with interstation distance, there is a slight decline as the subsystems move from Urban to High Speed. However, for Intercity and High Speed networks there is also a valley centered at flat gradient where the importance drops;

- The importance of efficiency again shows little difference between subsystems or gradient values, apart from the previously described increase for High Speed lines and services;

- Coasting limit and maximum speed exhibit similar trends, although that of coasting is more pronounced. As the gradient increases from steep downhill to steep uphill, the importance of these factors decreases. This rate of decline is much more significant as the subsystem moves from Urban to High Speed;

- The substantial decline in importance, at its worst point, brings coasting limit and maximum speed lower in ranking than all other factors.

The factor trends have been presented in an area chart using the same method as for interstation distance. However, due to the influence of gradient, this is solely a representation of the subsystem trends for factors and the effect of gradient should be borne in mind for factor ranking.

Average gradient μ* values for the energy KPI
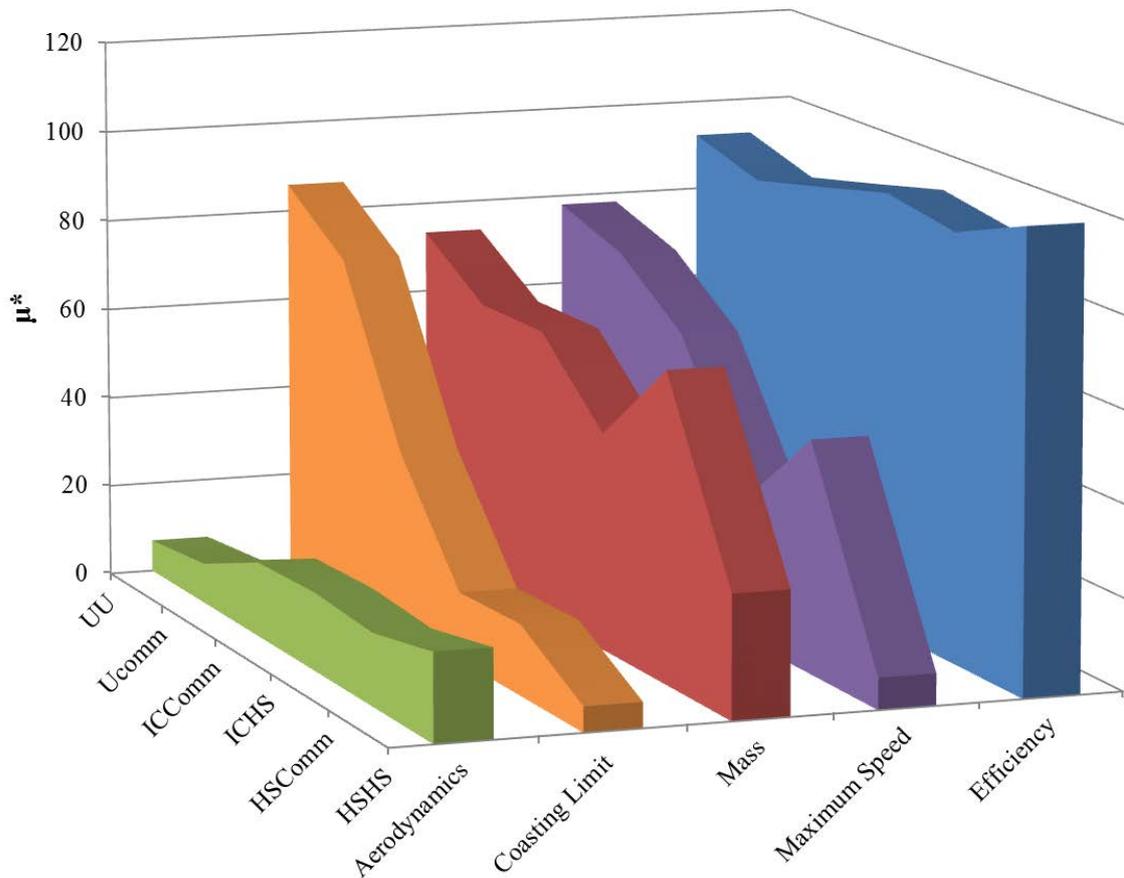
Figure 66: Area plot showing the key trends for the energy KPI based on the μ* gradient values

6.4.4 System Results Summary

The three approaches to presenting the results have given insight into the relationships between the subsystems, external factors, internal factors and energy. The original six subsystems can be assembled into three distinct groups based on their appropriate solutions: these are Urban networks, High Speed services running on High Speed routes, and Inter-city services and High Speed Commuter services. Overall, interstation distance has a minimal impact for all factors except the coasting limit and the change of coasting importance only affects some of the subsystems. It does not change the ranking of solutions for the first two groups. However, even for ICComm and HSComm services, where the ranking of solutions does change as interstation distance increases, the key and secondary factors remain the same. Generally speaking, coasting limit is more effective at reducing energy consumption for Urban systems and declines in effectiveness as the subsystems change through to High Speed.

The next main solutions for all subsystems are maximum speed followed by efficiency, although maximum speed drops in importance for High Speed services on High Speed networks.

The gradient profile of a route can have a significant influence on the ranking of the solutions for subsystems, particularly if a route has steep downhill gradients. In this case, the coasting limit and maximum speed are of significant importance. However, their ranking dramatically decreases as the gradient changes through zero gradient and to uphill. The remaining factors remain fairly constant, meaning that the next key factor is efficiency.

6.5 Chapter Summary

This chapter described the implementation of Stages 5-7 of the developed method, using the background information as presented in chapter 5. The results of each subsystem were discussed in detail individually, and PCA conducted on points of interest concerning the external factors of interstation distance and gradient. The PCA verified the initial Morris rankings, and helped to clarify the relationships between the key factors, energy and journey time. The Trend Identification Plot (TIP) was introduced as an effective way of determining the relationships between individual factors and the KPIs. Following the in-depth subsystem analyses, the relationships between subsystems were explored. Each of the three methods used allowed different information to be gleaned, building a detailed picture of the whole system. The tabular results offered an overview of the key factors and factor relationships in relation to the external factors. The heat maps allowed the relationships between subsystems in terms of suitable solutions to be identified easily, without being clouded by unnecessary information regarding the solutions themselves. Finally, the height maps gave a detailed overview of the relationships between the importance of each internal factor for each subsystem and external factor. In terms of the hypotheses, this chapter has allowed me to show that the appropriate solutions for railways do indeed differ depending on the network and service characteristics of the railway (as defined by the subsystems); that these differences can be used to determine the relationships between the subsystems; and that the results are capable of informing further experiments. The next chapter looks more in depth at efficiency, which was identified as a key solution for all subsystems.

Chapter Seven

In Depth Simulation: Efficiency Improvement

"Once we've made a decision, we are efficient only if we go through with it decisively, undistracted by doubts about its correctness"

<div align="right">J. Cleese (1991)</div>

7.1 Introduction

This chapter illustrates how the information gathered from the SA can be used to inform further simulations, as suggested in Method Stage 8. Efficiency was recognized as a key factor for all subsystems, meaning that improving the drive chain is a key solution. This supplementary investigation therefore concerns the feasibility of PMSM upgrades for all subsystems. Firstly new background information is introduced regarding railway traction systems and the motoring and braking characteristics of Induction Motors (IMs) and PMSMs, which is used to refine the STS simulation model. Simulation scenarios are then conducted for each subsystem, and the results used to perform a cost analysis.

The black italicised content in this chapter has been taken from Douglas et al., 2016c, in accordance with the IEEE publishing agreement in Appendix B.

7.2 Background

The rail energy SA introduced in chapter 5 and conducted in chapter 6 identified efficiency improvement as a key solution to reduce energy consumption for all railway subsystems. The system results also showed consistency in the importance of efficiency as a factor, regardless of the external factors of interstation distance and gradient, making it an excellent candidate for further study. The most feasible solution to improve the efficiency of the drive chain, as determined in Chapter 5, is the implementation of Permanent Magnet Synchronous Motors (PMSMs). *PMSMs are not only able to reduce traction losses but also increase regenerative braking capability and save energy through mass reduction. They allow the use of electric braking without requiring fully rated mechanical brakes for emergency use. PMSM technology is currently in operation around the world, mostly for metro and high speed*

operations, with studies showing savings of 5-20% (Douglas et al., 2015). Such a wide range highlights that energy savings greatly depend upon the vehicle, service and drive chains under consideration. Upgrading existing traction systems requires investment, particularly because of the increased number of inverters and protection needed (Kondo, 2010). Therefore, although the efficiency improvements afforded by PMSM technology are desirable across all railway types, any implementation must be considered in terms of cost-benefit. This cost analysis will also be important for ROSCOs procuring new rolling stock, who want proven technology, guaranteed performance and energy reduction.

This modelling study therefore aims to evaluate the introduction of PMSM technology to the previously defined railway subsystems*, considering not only the primary energy saving but the impact of regeneration and the investment cost compared to the current motors, in order to understand the feasibility of implementation for each subsystem in the first instance. As with the previous analyses, it should be recognised that the implementation of a solution on a real network would require a realistic model of the given network and the consideration of other factors, as every railway system is unique. These results are therefore only intended to give guidance on the suitability of PMSM technology for the different subsystems, to allow further simulations to be conducted. In order to evaluate the potential energy savings of upgrading the existing drive chains of each subsystem to PMSM technology, the current drive chains and the key differences between the current motors and PMSMs must be understood.

7.2.1 Railway Traction Systems

As discussed in Chapter 5, *the drive chain configuration of a vehicle changes dependent on the power supply of the network and power requirements. Urban rail systems are mostly electrified at 600 V, 750 V or 1500 V DC (Gonzales-Gil, et al., 2014), using either third rail or overhead line, while electrified Intercity and High Speed lines are powered using 25 kV AC from an overhead catenary. Although some railway rolling stock use DC traction machines, AC machines are preferred due to their less intensive maintenance regime, greater reliability and increased power density (Schmid and Goodman, 2014). Some rolling stock is dual supply, meaning it can use either DC or AC supplies, which are switched in using circuit breakers. The supply is converted, via line filter for DC or transformer and rectifier (four quadrant converter) for AC, to create the DC link (Baliga, 2015). This DC voltage then: feeds the machines via a Variable Voltage, Variable Frequency (VVVF) inverter; supplies the vehicle*

auxiliaries after further filtering and conversion; and is connected to the rheostats that dissipate braking energy. A block diagram of the traction chain is shown in Figure 67, with the efficiencies of each block denoted. References for these values are provided in Table 32. Figure 68 shows the circuit diagrams of each of the relevant blocks. It is assumed that all power converters (rectifier, inverters and appropriate auxiliary converter) use Insulated-Gate Bipolar Transistor (IGBT) devices. In this study, the conventional machines are replaced with PMSM technology, which significantly increases the motor efficiency. As the inverters would also need to be replaced for PMSMs, the simulated IGBT inverters are upgraded with Silicon Carbide (SiC) devices, which represent the latest technology (Brenna et al., 2014).

Table 32: Efficiencies of drive chain components (Douglas et al., 2016c)

Component	Efficiency	Reference
Line Inductor	0.99	
Auxiliary Supply System	0.95	(Hoffrichter et al., 2012; Wang et al., 2013)
DC Smoothing	0.995	(WIMA, 2011)
Transformer	0.95	(Hoffrichter et al., 2012; Steimal, 2014)
IGBT Power Converters	0.98	(Kondo, et al., 2014; Steimel, 2014)
Silicon Carbide Power Converters	0.99	(Brenna et al., 2014)
AC Induction Motors	0.94	(Gonzales-Gil, et al., 2014)
PMSMs	0.97	(Kondo and Shimizu, 2008; Toshiba, 2015)
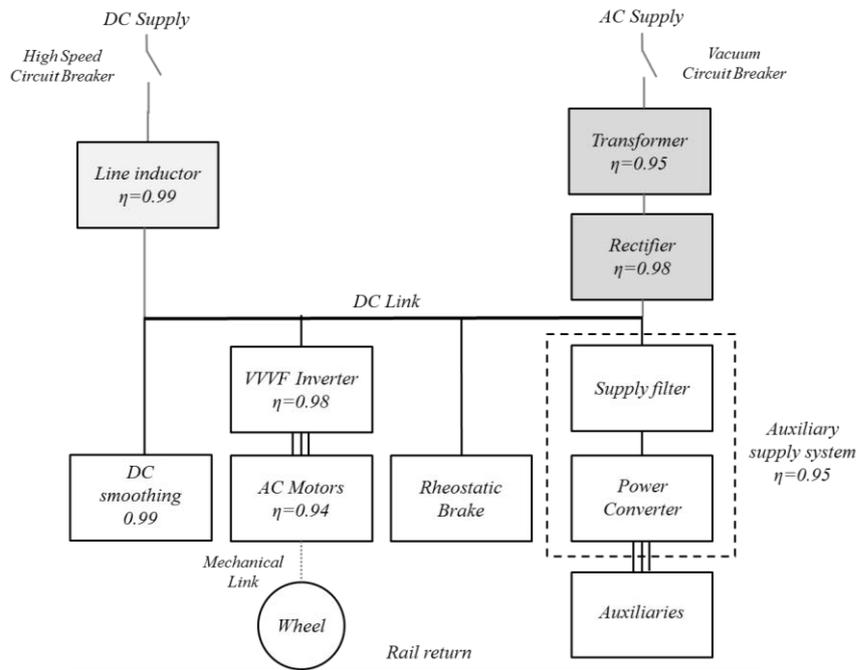
Figure 67: Traction conversion chain block diagram, with block efficiencies, for dual voltage supply (Douglas et al., 2016c)

The drive chain and regeneration efficiencies for DC and AC supplies powering either AC Induction Motors (IMs) or PMSMs are given in Table 33, and have been calculated using the

values from Table 32. It is assumed that all components have the same efficiency for current flowing during traction and electric braking. This means that the value for regeneration to the line is the same as the drive chain efficiency. It was previously stated that between 10-15% of traction energy is lost in the drive chain. As the calculated efficiencies fall within this limit, it can be assumed that the individual efficiency values used are reasonable.
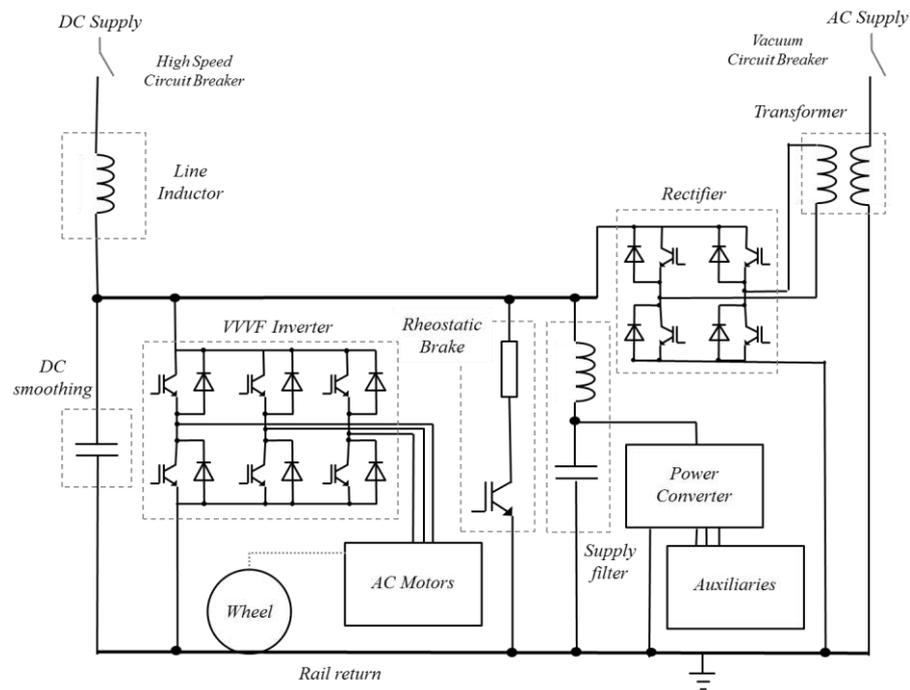
Figure 68: Traction diagram for dual voltage supply showing main circuit components (Douglas et al., 2016c)

Table 33: Transfer efficiencies for traction and regenerative braking (Douglas et al., 2016c)

Power Supply	DC		AC	
Motor Technology	*Induction Motors*	*PMSMs*	*Induction Motors*	*PMSMs*
Drive Chain efficiency	0.903	0.941	0.858	0.894
Regeneration to the auxiliaries	0.875	0.912	Same as DC	

7.2.2 Motoring and Braking Characteristics

One of the key differences between IMs and PMSMs is their motoring and braking characteristics: these must be included in order to simulate PMSM upgrades successfully. *Typically, the force (torque) provided by the motors of a railway vehicle at a given speed is described by the Tractive Effort (TE) curve. Traction motors provide a constant TE at low speeds, as the power delivered increases to its maximum value. Once the maximum power has*

been reached, the constant power region is entered and the force provided by the machines decreases, according to the equation $P = Fv$. This is illustrated in Figure 69.
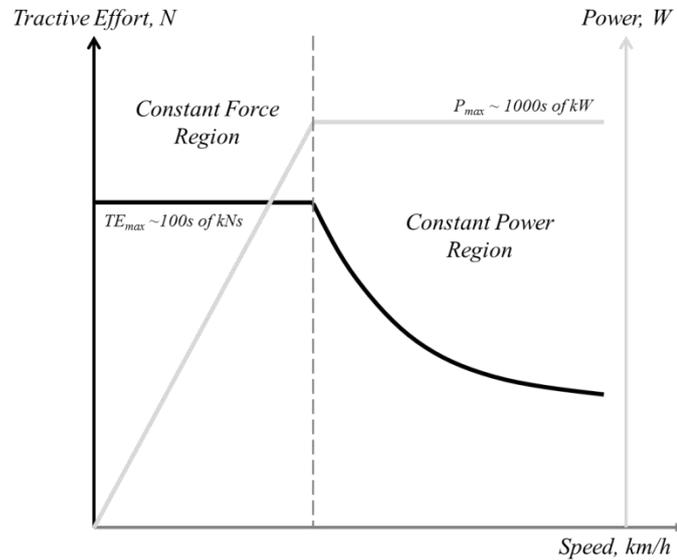
Figure 69: Tractive effort and power curves for railway vehicles (Douglas et al., 2016c)

Traditionally, the maximum Braking Effort (BE) of a vehicle was determined by the mechanical braking system, however, electric machines allow for dynamic braking and subsequent regeneration to the line, if it is receptive. The braking characteristic differs from the TE curve as it does not provide full effort at low speed, but instead decreases linearly (Cole, 2006). The constant force region typically extends beyond that of the TE curve, by approximately 70% (RSSB, 2008). The extension occurs because the motor losses are an advantage in the reverse direction. When the braking need cannot be met by the electrical braking system, the remaining braking force is applied using the mechanical braking system. *The typical braking characteristics for an Electric Multiple Unit (EMU) are shown in Figure 70. The TE and BE curves for PMSMs are generally very similar to those for IMs. However, for the same weight and volume, PMSMs can deliver increased power and TE compared to their IM counterparts. A set of ratios, Figure 71, have been devised to emulate the differences in tractive effort and braking characteristics between IMs and PMSMs for the study, using findings from the Green Train Project (Soulard, 2012) and personal communications (Neubauer, 2016).*

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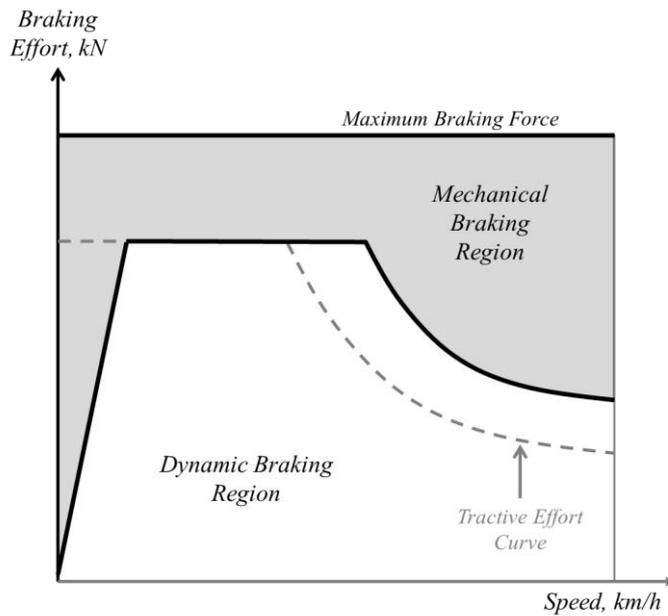
Figure 70: Typical mechanical and dynamic braking characteristics for an Electric Multiple Unit (EMU) (Douglas et al., 2016c)

The maximum torque provided by the PMSM is approximately 30% greater than that of the IM, and the constant power region also extends by 30%. As previously stated, the constant force BE for IMs is about 70% greater than the TE. However, for PMSMs this effect is slightly lower due to reduced field weakening. PMSMs are also able to apply electric braking at lower speeds than IMs.
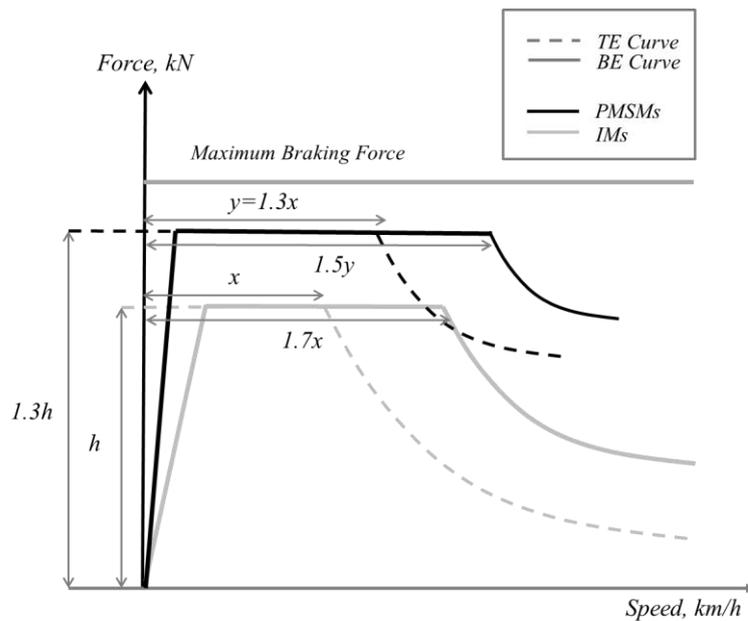
Figure 71: Ratios for the TE and BE curves for PMSMs and IMs (Douglas et al., 2016c)

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7.3 Simulation Model and Methodology

The Single Train Simulator (STS) is used to conduct the simulations necessary to complete this investigation. *For each of the subsystems the energy consumption is first calculated for the traditional subsystem drive chain configuration and then for the PMSM upgrade.* The impact of regeneration is investigated by considering the energy consumption if the line is both non-receptive (no regenerated energy is used) and fully receptive (all regenerated energy is used). In both of these cases it is assumed that the regenerated braking energy primarily feeds the on-board auxiliaries. The line can be fully receptive if reversible substations are used which, by their very nature, AC substations are. This is therefore not an unreasonable test case for Inter-city and High Speed networks. For Urban networks, which are DC powered, direct feedback to the grid is not possible without upgrading the substations. However, as there are more trains operating closer together there is a greater opportunity for the exchange of energy between trains in a section, which can be improved by synchronising the timetable of braking and accelerating trains. If the study shows that PMSM upgrades are feasible, then further analysis would be needed to evaluate the true receptivity of the line for the appropriate subsystems.

The efficiencies of each drive chain configuration are simulated by controlling the generation rate as described previously in Chapter 5. However, since braking energy is fed into the auxiliaries the regeneration rate cannot be used as before. Instead, for each distance step during which the train brakes, the total energy requirement of the auxiliaries is calculated and the regenerated energy - taking into account the efficiency of regeneration to the auxiliaries - is used to meet this requirement. If any energy remains, it is fed back to the line using the appropriate efficiency, effectively offsetting some of the traction energy drawn from the supply. This is illustrated in Figure 72.

The motoring and braking characteristics of the PMSMs are calculated using the ratios on the previous page and the initial IM TE and BE curves for each subsystem vehicle. It is assumed therefore that the PMSMs are the same size and weight as their IM counterparts. In reality, a PMSM of the same power rating would be used, reducing the mass and bringing about further efficiency improvements. In order to simulate this detailed information for each subsystem concerning the size and mass reductions, thermal environment, cooling requirements; and thermal constraints would be required. This information is not only difficult to obtain but adds

unnecessary complexity. In practice, the tractive effort diagrams for different machines vary depending on their design application anyway, meaning that the general rules described are necessarily approximate. However, for the purpose of this study, such an approximation is appropriate as it allows a general comparison between subsystems to be made.
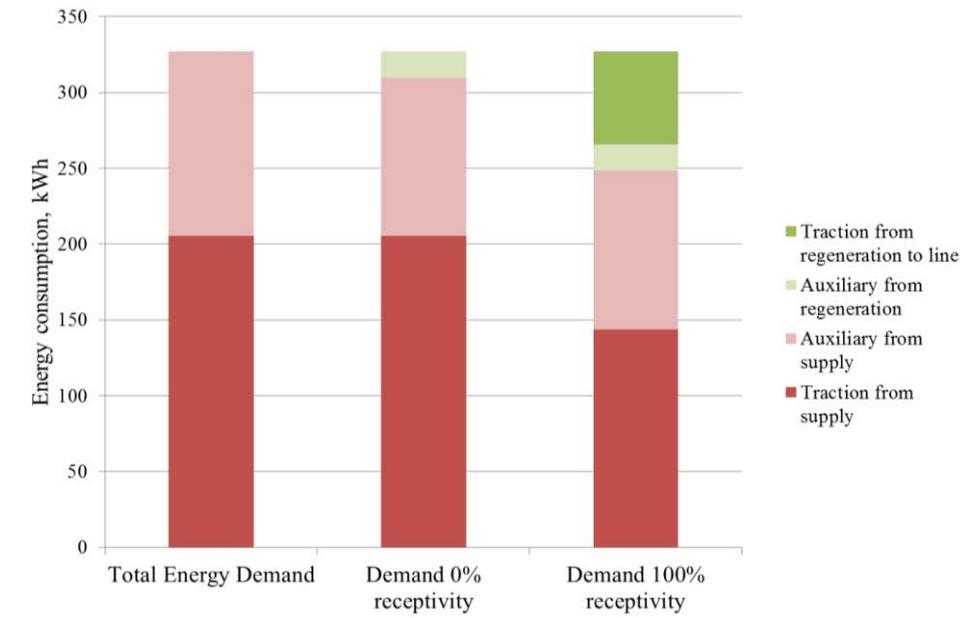
Figure 72: Breakdown of energy consumption for UComm subsystem using IMs, relative to the line receptivity (Douglas et al., 2016c)

The key parameters for each subsystem vehicle are given in Table 34, including acceleration rate, braking rate, auxiliary power requirements, the ratio of powered axles and number of motors. Table 35 gives the relevant network and service requirements for each of the subsystems, which are based on the previous analysis.

Table 34: Key parameters for each of the subsystem vehicles (Douglas et al., 2016c)

Network	Urban		Inter-city		High Speed	
Power Supply	750V DC		25kV AC			
Service	Urban	Commuter	Commuter	High Speed	Commuter	High Speed
Mass, tonnes	100	104.0	120	600	270	790
Power, MW	1.12	1.10	1.2	5.95	3.49	12.24
Max. Speed, km/h	80	100	120	200	160	300
Acceleration, ms^{-2}	1.1	1.0	0.8	0.30	0.7	0.35
Service brake, ms^{-2}	1.2	1.1	0.9	0.5	0.9	0.5
Auxiliary Power, MW	0.25	0.25	0.25	0.75	0.50	1.50
No. of passengers	400	400	240	590	350	1,000

Number of cars	3	3	3	9	6	16
Ratio of powered axles (Phillips, 2011)	100%	67%	67%	50%	67%	50%
No. of motors	12	8	8	18	16	32

Table 35: Specific service requirements for each subsystem (Douglas et al., 2016c)

Network	Urban		Inter-city		High Speed	
Service	Urban	Commuter	Commuter	High Speed	Commuter	High Speed
Service Distance, km	20	30	60	250	100	210
Interstation Distance, km	1	3	12	50	25	70
No. of stations	20	10	5	5	4	3
Number of cars	3	3	3	9	6	16
Dwell Time, s	20	40	60	120	120	240

7.4 Results

The initial results in Figure 73 show that when the line is not receptive, there is minimal difference between the energy consumption using PMSMs compared with IMs. In fact, the traction demand actually increases slightly, due to the increased vehicle power. However, this increased power provides greater acceleration, thus shortening the journey time (Figure 74) and reducing the auxiliary demand, meaning that the energy consumption is approximately the same. When the line is receptive, the savings vary from 3% to 11%, depending on the railway subsystem. Urban services achieve the highest savings, which is likely due to the frequent braking. Braking forms a large proportion of their trajectories meaning that they take more advantage of the extended braking characteristic of PMSMs than other services. This relationship between braking frequency and saving is supported by the fact that Commuter services on a network save more than the respective High Speed service. However, High Speed networks outperform Intercity because of their longer braking duration, which commences from higher speeds.
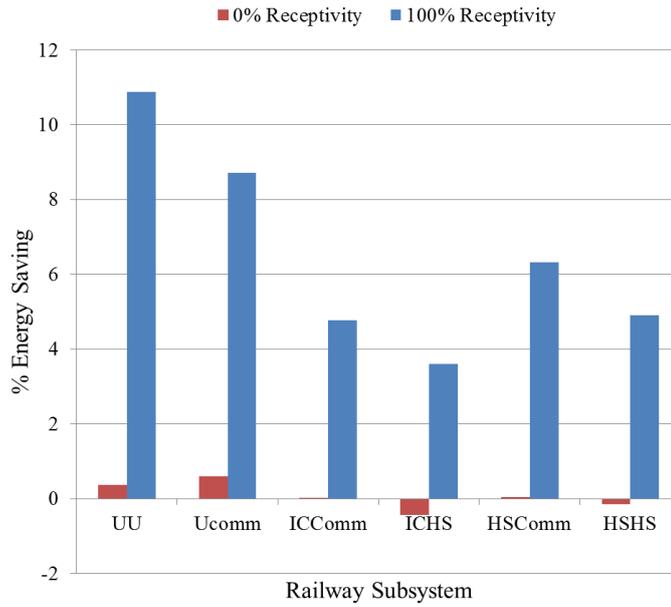
Figure 73: Percentage energy savings for each subsystem when the motors are upgraded (Douglas et al., 2016c)
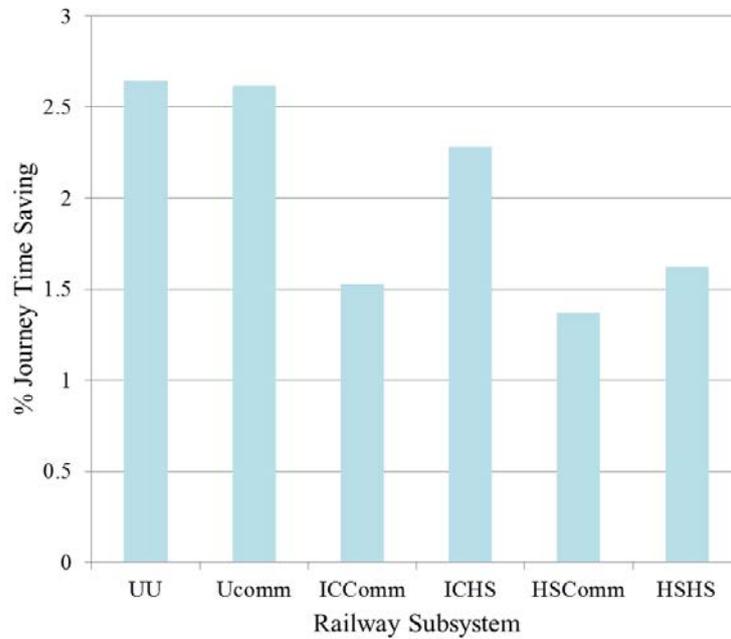
Figure 74: Percentage journey time savings for each subsystem when the motors are upgraded (Douglas et al., 2016c)

Another way to look at the results is to calculate the saving per passenger km, as shown in Figure 75. When considering information in this form, both Urban and High Speed networks achieve better savings than Intercity, although Urban services still achieve the greatest benefit.

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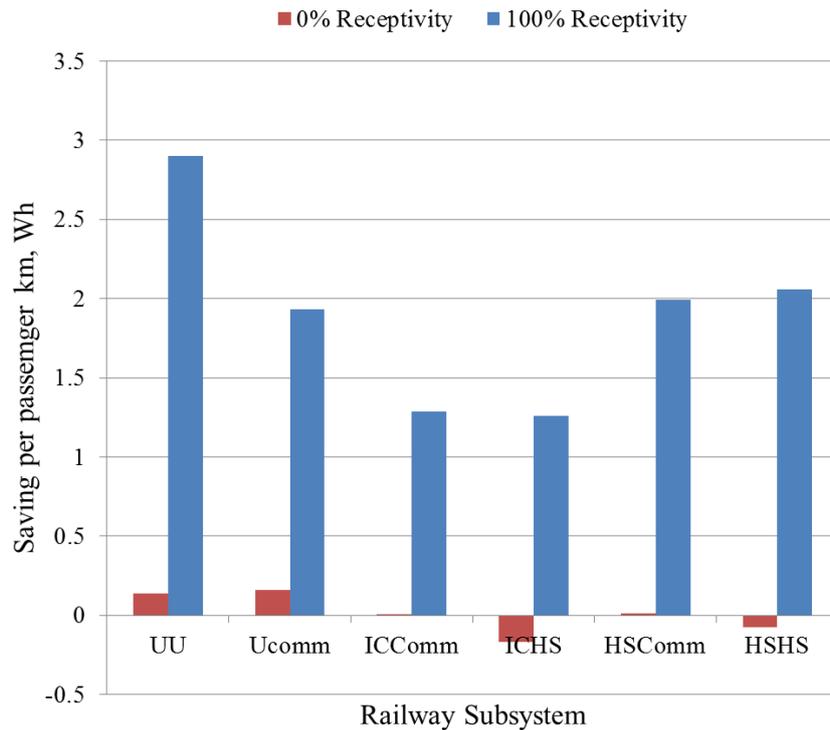
Figure 75: Saving per passenger km for each subsystem when the motors are upgraded (Douglas et al., 2016c)

In order to determine the feasibility for implementation of PMSM technology, the energy savings must be considered against the cost of the upgrade. A preliminary analysis was conducted based on the payback period – a common measure for upgrades. If the money for the upgrade can be recuperated within a reasonable period then it can be considered commercially viable. In the case of railway traction chain upgrades, this 'reasonable' period depends on the expected remaining lifetime of the rolling stock. The payback period is only calculated for the case of 100% receptivity, as costs cannot be recovered through energy savings when the line is unreceptive.

The calculated payback periods in this study may be considered to be conservative estimates. In reality, an upgrade of this type would provide wider benefits in terms of reduced maintenance, greater utilisation and even increased revenue from better service provision. In the case of urban services, further payback could be attained as less braking energy is dissipated, reducing the need for cooling in tunnels. A full economic analysis would need to take all of these factors into consideration and would probably calculate shorter payback durations for each type of service.

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The payback period is calculated as follows:

$$Payback\ Period = \frac{Upgrade\ Cost}{Cost\ Savings\ per\ year}$$

$$Payback\ Period$$
$$= \frac{Cost\ per\ motor * No.of\ motors}{Saving\ per\ journey(kWh) * No.of\ journeys\ per\ year * Cost\ per\ kWh}$$

$$No.of\ journeys\ per\ year$$
$$= \frac{Daily\ service\ operation\ hours}{Service\ journey\ time} * No.of\ days$$

Note that the calculation for this payback period is not discounted. A discounted payback period could be used to take into account the time value of money.

Primarily, it is assumed that each service operates for 15 hours a day, 350 days a year. The price per kWh is taken as 8.368p, which is the tariff dictated in EC4T (Fullard, 2015), and the average upgrade cost per motor as £30,000 (Neubauer, 2016). Figure 76 shows the results using these assumptions. From this figure, it can be read that High Speed services running on High Speed networks are the best candidates for efficiency improvements, as upgrades can be recuperated in less than 6 years. However, the highest payback periods (for intercity services) are still less than 18 years which is not an unreasonable duration, taking into account that rolling stock life usually exceeds 35 years.
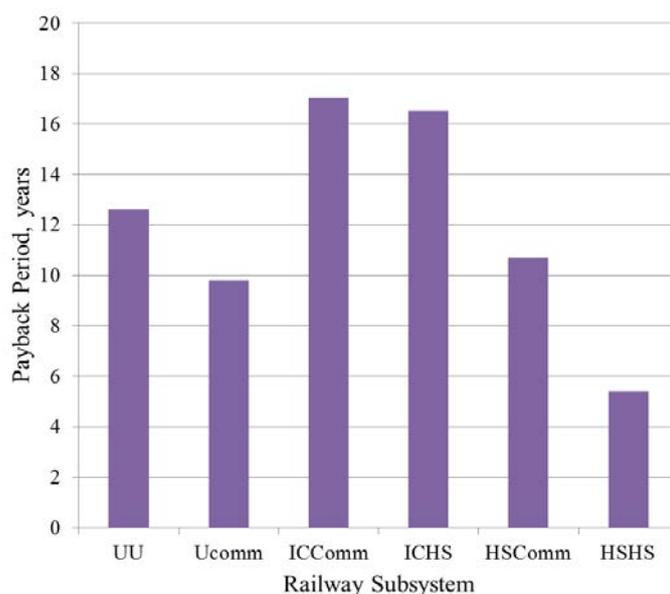
Figure 76: Payback period assuming fixed operational hours and motor costs between services (Douglas et al., 2016c)

In reality, the hours of operation and price per traction motor for each of the services are likely to differ. In general, urban services operate for a longer proportion of the day, with some operators now running services 24 hours a day (Volterra, 2014). Table 36 shows the typical hours of operation and number of journeys performed each day by each service vehicle (these were determined by looking at current timetables for a representative service of each type). Most operators stop services before midnight, which limits the operational hours of High Speed services in particular. In order to arrive at their final destination before this cut off their last departure must be early enough to account for the journey time. The cost of each motor will also differ depending on the power requirement. Assuming a minimum price of £28,000 and a maximum of £45,000 (Neubauer, 2016), the motor cost has been scaled according to size, also shown in Table 36.

Table 36: Revised operational hours and motor costing for each subsystem (adapted from Douglas et al., 2016c)

Network	Service	Hours of operation	Number of journeys	Motor Power kW	Motor cost, £k
Urban	Urban	20	41	93	28,000
	Commuter	18	36	138	34,097
Inter City	Commuter	17	26	150	34,675
	High Speed	11	6	331	42,685
High Speed	Commuter	18	22	218	37,701
	High Speed	15	14	383	45,000

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Figure 77 shows the payback period considering revised operational hours and motor cost, using the standard payback period calculation. Scaling the traction motor cost and inputting realistic operational hours has reduced the payback period for the majority of services, most notably Urban services. However, both Urban and High Speed networks show great commercial viability for such an investment, being able to pay back the upgrade cost in 10-15 years. The payback periods for the investments are based on the current energy tariff set by Network Rail, which is a little over 8p per kWh. As demand for energy increases, it is possible that this cost will increase, reducing the payback period further. Figure 78 illustrates the effect of increasing the price per kWh by between 1 and 3p.
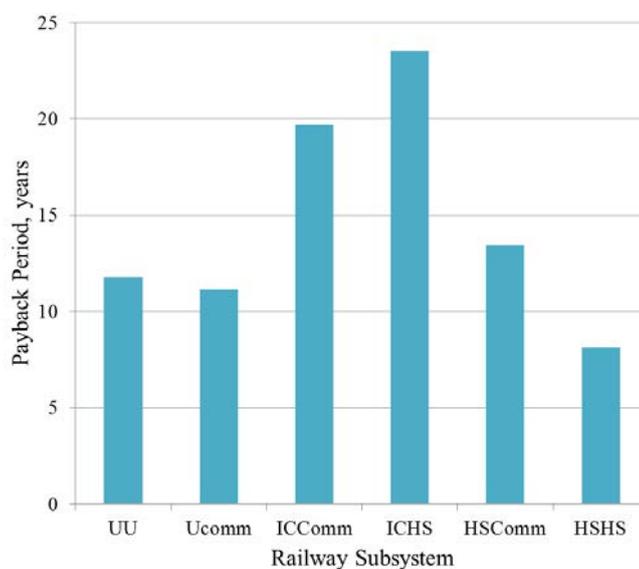
Figure 77: Payback period assuming operational hours and motor costs as shown in Table 36 (adapted from Douglas et al., 2016c)
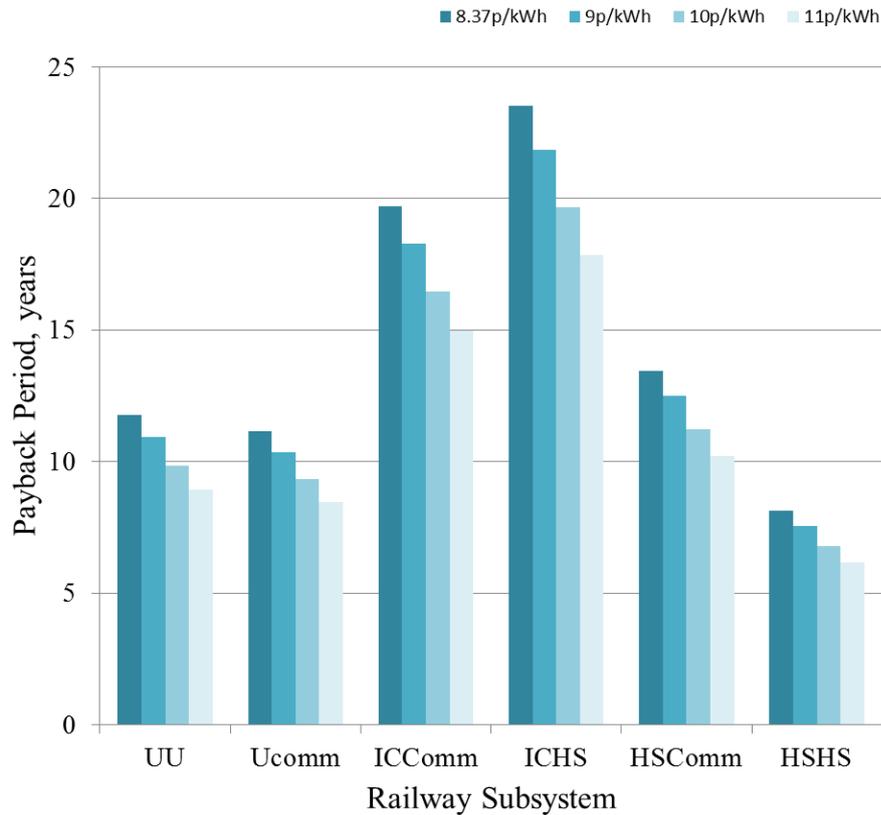
Figure 78: Payback period for increased energy costs per kWh (adapted from Douglas et al., 2016c)

7.5 Conclusions

The results of this in-depth simulation *have given indication of where PMSM technology is most viable, based on the estimated energy savings and traction motor cost. Using motors of the same size and volume, energy and cost savings cannot be achieved on a service without using regenerative braking, due to the increased power requirement. An area for future investigation is therefore whether or not savings can be achieved in this instance by upgrading IM motors with PMSM not of the same size, but of equivalent power. This assessment would be more complex as it would require calculating the new size, weight and cooling requirement of the motors for each subsystem. However, it is expected that energy would be saved if cooling requirements and weight are reduced. When regenerative braking is considered with motors of the same weight and size, the energy savings vary from 3 % to 11% depending on the subsystem, with Urban being the most worthwhile. Calculation of the payback periods, based on motor cost and operating hours, show that both Urban and High Speed networks receive a valuable benefit from an upgrade, and are able to recover the initial*

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costs in less than 15 years. However, even Inter-city networks can recover costs in less than 25 years which is not unreasonable. There are further benefits to installing PMSM technology including reduced maintenance, journey time benefits and the possibility to downgrade the mechanical braking systems, due to the increased integrity of PMSM dynamic braking. When these factors are also taken into consideration, the payback period is likely to reduce even further, making upgrades even more attractive.

7.6 Summary

This chapter has provided an example of how the SA findings for the rail energy application may be used to inform further studies. Based on the efficiency results, the feasibility of implementing PMSM technology on each railway subsystem was investigated and a cost analysis conducted. In order to conduct the simulation, the generation and regeneration efficiencies of typical AC and DC traction chains were calculated; and general ratios defined to simulate the difference in motoring and braking characteristics between IMs and PMSMs. The STS, as previously introduced, was upgraded to incorporate this new information. The energy saving results with and without regeneration were used to conduct a cost analysis and determine the approximate payback periods for each railway subsystem if PMSM technology was introduced. The payback time ranged from 15-25 years for a fully receptive network, using current energy prices. Considering the other benefits and rising cost of energy, this period is a conservative estimate which ultimately showcases the potential of PMSMs to save energy and reduce costs in railway networks.

Chapter Eight

Conclusions

"This is not the end. It is not even the beginning of the end. But it is, perhaps, the end of the beginning."

<div align="right">W. Churchill (1943)</div>

This research set out to develop a method to find solutions for complex optimisation problems. In order to do so research was conducted into complex systems, the current approaches to solving complex problems, and multi-variate data analysis and visualisation, as set out in Objectives 1 and 2 in the Introduction Section 1.2. The method was then developed, taking into consideration how subsystems of systems were defined, how the suitability of solutions was to be determined, which data should be captured in the method and how it was to be kept consistent between subsystems. To demonstrate the suitability of the screening method, and meet the final Objective, the developed method was then applied to the problem of saving traction energy in rail.

8.1 Research Hypotheses

The three research sub-hypotheses cover the key aims of the method which are: to find the best solutions for subsystems; to understand the relationships between subsystems; and to determine appropriate areas for further experimentation. Each of the hypotheses below relates the method aims to the specific example of saving traction energy in rail, in order to demonstrate proof of concept.

- Do the appropriate solutions for particular railways differ depending on the network and service characteristics of the given railway?

In order to conduct the sensitivity analysis that forms the core of the developed method, railways were categorised into six subsystems based on their network and service characteristics, as detailed in Chapter 5 Section 3. Three network and service types were identified: these are Urban, Inter-city and High Speed; and Urban, Commuter and High Speed respectively. Only 6 subsystems exist because High Speed services do not run on Urban

networks and vice versa. Six solutions to save traction energy were also identified within Chapter 5 as being feasible for implementation on the railway. In Chapter 6, these solutions were investigated for each subsystem using the Morris method of sensitivity analysis, by mapping each solution to an input factor. The impacts of solutions were evaluated against the two KPIs of energy and journey time. In Section 4, the initial Morris results for each subsystem, for each of the external factors (interstation distance and journey time) were plotted, giving indications as to points of interest for further analysis. PCA was then used to provide further insight into the relationships between the factors themselves, the KPIs and the external factors at these specific points. The Trend Identification Plot, a scatter plot of the KPI results coloured according to the values of a particular factor, was introduced as a novel way of visualising the relationship of a single factor at a time.

The results analysis in Chapter 6 Section 4 indicated that the most appropriate solutions do differ between railway subsystems, and are linked to by their network and service characteristics. The external factors of interstation distance and gradient also affect the suitability of solutions and can have some impact on the relationships between factors. These results demonstrate that partitioning the system into subsystems using quantifiable factors is a good approach. The analysis has allowed me to give detailed recommendations for each subsystem in turn, which may have been missed in a whole system analysis.

- Can these differences be used to determine the relationships between the different networks and services?

The results for the whole system were presented in Chapter 6 Section 4 in three different representations: tabular, heat map visualisations and surface visualisations. The heat map visualisations were created by assigning a unique number to each set of factor results for a given interstation distance or gradient, using simple numerical encoding. These resulting figures offered a concise overview of the differences between systems without being clouded by the individual factor trends or importance. Based on the maps, three groups emerged, namely the Urban network, High Speed High Speed subsystem, and Inter-city network and High Speed Commuter services respectively. Therefore, the heat maps alone represent a way to determine the relationships between the different networks and services, thus meeting the sub-hypotheses. However, additional information was gained from the surface visualisations,

which provided greater clarity regarding the overall factor trends in relation to the subsystems and external factors.

- Can the results be used to inform further experiments?

A simple answer to this question is 'yes'. Based on the consistency of efficiency as a key factor for all subsystems, an analysis of PMSM implementation was conducted in Chapter 7. This investigation focused on assessing where PMSM would be most suitable for implementation in terms of the previously defined subsystems, using a simple cost analysis. The analysis showed that replacing traditional IMs with PMSMs of the same size and weight was feasible in terms of cost-benefit, if the line was receptive to regenerative braking. Urban and High Speed networks were particularly responsive, with both being able to recuperate the installation cost within 15 years. This analysis was limited, as it assumed full line receptivity to regenerative braking, which is not possible for Urban networks without reversible substations; and did not include the secondary benefits of PMSM such as reduced maintenance costs and faster journey times. However, it did generally indicate where PMSM technology would have the greatest benefit, leading the way for further simulations.

8.2. Key Achievements

This research has resulted in a number of key achievements:

- I have developed a screening method to assess solutions for complex optimisation problems;

- I have successfully applied the method to the problem of traction energy saving in rail

    - Partitioned the railway into six subsystems based on quantified network and service characteristics;

    - Evaluated traction energy saving solutions in terms of feasibility, and selected six solutions for investigation;

    - Introduced a simple approach to determine the number of Morris trajectories needed for an evaluation;

- o Identified the most suitable solutions for each subsystem, dependent on the external factors of interstation distance and gradient;

- o Investigated the relationships between factors using PCA;

- o Introduced the Trend Identification Plot as a simple way of visualising the relationship between each factor and the KPIs;

- o Introduced the encoded heat map as a way of comparing the subsystem results at system level;

- o Determined relationships between the subsystems based on the suitable solutions.

- I have conducted an in-depth study to determine the suitability of PMSM technology for different subsystems, based on the SA results

  - o Found that PMSM are most suitable for Urban and High Speed networks;

  - o If the line is receptive, the approximate payback period is between 10 and 15 years.

8.3 Recommendations

In terms of the railway traction energy saving application, a number of general recommendations can be made as to which solutions should be investigated:

- For Urban and Inter-city Commuter subsystems with short interstation distances, both coasting speed and maximum speed are critical factors affecting energy consumption. Therefore the development of energy-efficient trajectories for these subsystems is recommended. It is important that drivers are able to implement these trajectories, which may require the development of intuitive Driver Advisory Systems.

- For High Speed trains running on dedicated networks, the key to energy saving is drive chain efficiency. Reducing the operating speed may also be an appropriate solution. However, if the object of the service is reduced journey times, this may be

unsuitable. Aerodynamic improvements can also have some effect and should be incorporated at the design stage, where possible.

- Drive chain efficiency improvements indicated significant savings across all subsystems and a preliminary cost-benefit analysis proved that the installation of PMSM was feasible across all subsystems. It is recommended that further work be undertaken in this area to determine the possible savings using equivalent power motors, rather than equivalent size and weight, and determine whether this yields benefits even for lines which are non-receptive to regenerative braking.

- For Inter-city Commuter trains with longer interstation distances (>10 km) as well as generally improving efficiency and reducing maximum operating speed, there is the opportunity to save energy through design. These trains in particular are responsive to improvements in both aerodynamics and mass, and it is recommended that such improvements are investigated in detail to be implemented at the design stage.

- The gradient profile of a network has shown a significant impact on the ranking of solutions. It is therefore recommended that the impact of gradient is investigated in detail, using routes that incorporate both uphill and downhill sections. However, this is only likely to impact Inter-city networks, due to their operation over long distances on legacy infrastructure. Services operating on both Urban and new dedicated High Speed networks are less likely to encounter steep gradients, although, if there are instances where they do occur, their impact should be investigated.

These are a snapshot of the recommendations that can be made at high level. Based on the individual trends in each subsystem, it is possible to make more detailed recommendations for sections of subsystems. These can be determined by referring to the individual subsystem results and analyses.

8.4 Further Work

This work has opened up a number of different research opportunities:

- In the first instance, it would be interesting to apply the method to an optimisation problem in another field to determine its suitability in other contexts. Of particular

interest would be the application to a problem outside of the railway domain, or engineering altogether. I would be curious to know whether the approach can be translated to fields that primarily use qualitative assessments, and how the translation from qualitative to quantitative could be achieved.

- Another interesting consideration is what the results would be if another variance based technique, such as Sobol, were used in place of Morris. Although there is unlikely to be any differences in the conclusions, there may be representation techniques more suitable for the Sobol analysis, or differences in terms of computational requirements and calculation time.

- In terms of the railway traction saving application, a number of avenues for research have been uncovered. In-depth simulations of the appropriate solutions for each subsystem could be completed as detailed in Section 8.3, in order to find the optimal solution for a given network, or to gain further understanding regarding the external factors of interstation distance and gradient. An analysis based on the developed method was conducted solely for Urban networks (Douglas et al., 2016b) considering factors inherent in these systems, such as proportion of the line in tunnels and clustering of stations. The investigation of coasting would be of particular interest due to its high importance for Urban networks and its much lower relevance for High Speed networks.

- Another clear investigation was raised by the PMSM implementation. This is to evaluate the cost-benefit of PMSM technology based on motors of the same power capability, rather than the same size and weight. As previously mentioned, this adds complexity in terms of reduced weight, cooling requirements and changes in the thermal environment.

The purpose of this research was to develop a formal screening method to evaluate solutions for complex optimisation problems. The application of the method to the problem of traction energy saving in rail has demonstrated its suitability to provide information regarding: (i) the most appropriate solutions for each subsystem of the system, (ii) the relationships between the individual factors within a subsystem, (iii) the relationships between the subsystems themselves, and (iv) which areas should be considered for further experimentation. The

method provides a defined approach to discover important information about a complex system that is reusable and formalised, thus providing a clear starting point and direction for complex optimisation problems, which is currently lacking.

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Appendices

Appendix A: Publication First Pages
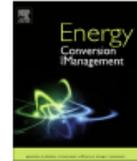
Review

An assessment of available measures to reduce traction energy use in railway networks

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ABSTRACT

Rail is becoming an increasingly popular choice to satisfy transportation demands locally, nationally and internationally, due to its inherent efficiency and high capacity. Despite this, operators are facing pressure to reduce rail energy consumption to meet efficiency targets, whilst still maintaining service quality and managing increased demand. A number of individual measures have been proposed to reduce energy in the rail sector, often showing good results on specific case studies. It is generally agreed that the attainable savings of a given measure change dependant on the route, vehicle and service characteristics. However, there is little information in the literature specifically regarding which measures are most suitable for given network types, or how they interact. This paper therefore aims to begin evaluating the available measures in terms of their suitability for different systems. Firstly, networks are defined in terms of their distinguishing features. As traction accounts for the majority of all energy use in the rail sector, the traction flow through a vehicle is considered as the starting point for an evaluation of measures. Current technologies and procedures are reviewed and categorised based on which area of traction use they target. Thought is given to the factors that affect implementation and the networks where they are applied. A key output of this paper is a comparison of the achievable energy savings of different measures dependent on the network type. It is hoped that this will provide a good starting point for identifying which measures are most applicable for a given network, and the characteristics that affect their success.

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Contents

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Method to evaluate solutions for complex systems: rail energy

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Many solutions have been developed to reduce energy consumption in rail, covering the three main areas of rolling stock, infrastructure and operations. These solutions often show significant energy savings in theory, simulation and practice. However, the success of a solution can only be evaluated within the scope of the study performed, which is limited to specific case studies. Because railways vary greatly, a solution deemed effective when applied to one railway may not be well suited to another, due to inherent differences. This work therefore aims to develop a method to evaluate solutions for complex systems, using energy saving in rail as an example. Distinct subsystems are quantitatively defined by determining the factors that make them unique. For rail, these are categorised into route, vehicle and service characteristics. Next, key performance indicators are identified that relate to the success of solutions. Finally, a sensitivity analysis is performed to evaluate which factors influence solution success for each subsystem. In-depth simulations of solutions can then be completed. The developed method is used to find the most influential factors when considering energy-saving solutions applicable to single trains, for six types of railway subsystems, using Morris' elementary effects method of sensitivity analysis.

Notation

a	acceleration
F_R	resistive force
F_S	propulsion force
M	mass
M_E	inertial mass
v	speed
W	resistive forces
λ	constant allowing for rotating parts

1. Introduction

Rail has been identified as an essential transport mode for an environmentally sustainable future, due to its inherent efficiency. By 2050, it is intended that rail will transport the majority of medium-distance passengers and up to 50% of current road freight over 300 km (EC, 2011). But, while expanding, the sector also has to meet internationally set energy and greenhouse gas emission targets (EC, 2010). The Railway Technical Strategy (RTS) (TSLG, 2012) has been developed to guide the rail industry in Great Britain to achieve both growth and efficiency, by broadly describing a number of solutions to increase capacity and reduce energy use, through a whole-systems approach.

Many of these solutions have previously been considered in research and tested in theory, simulation and practice, but a solution can only be evaluated within the scope of the study performed. This is often limited because most studies focus on the implementation of a single solution to a small number of specific case studies. However, railways are unique systems defined by a variety of factors, any of which could influence the effectiveness of a solution. To optimise energy saving across a whole railway, knowledge of which factors affect solution success for each system is needed, so that appropriate solutions can be implemented where they are most suited, maximising the energy saved.

This work uses the problem of identifying appropriate energy-saving solutions in rail to develop a method for evaluating solutions of complex systems. To minimise the complexity of the initial method development, the scope is limited to the following.

- Solutions to reduce traction energy use only. According to the Office of Rail Regulation (ORR, 2012) this accounts for between 80% and 90% of the energy used in rail, with the remainder consumed in stations, depots and so on.
- Solutions that can be applied to individual trains. This is useful as a primary study, to gain understanding of the effect of basic factors. When multiple trains are simulated, the interactions among them must be considered, which introduces complex factors such as the number of trains per hour, signalling type and homogeneity of stock.

Evaluation of Permanent Magnet Motor Energy Saving Technology for Different Types of Railways *

Heather Douglas, Felix Schmid, Clive Roberts and Stuart Hillmansen

Abstract— the majority of drive chain losses in railway vehicles are attributable to motor inefficiency. An attractive solution to reduce these losses, and the associated energy consumption, is the implementation of Permanent Magnet Synchronous Motor (PMSM) technology. PMSMs are not only more efficient, but smaller and lighter than traditional induction machines, which can further benefit energy saving. However, introducing this technology and the associated control systems can be expensive and complex. Therefore, in this study, the authors evaluate the cost benefit of introducing PMSMs into different railway sub-modes to see where this solution is most appropriate, in terms of energy saved. The impact of regenerative braking on the cost is also considered, by simulating dynamic braking characteristics and the receptivity of different systems.

Method for validating the train motion equations used for passenger rail vehicle simulation

Heather Douglas, Paul Weston, David Kirkwood, Stuart Hillmansen and Clive Roberts

Abstract

Train simulation software is conventionally validated by checking simulation results against equivalent data collected from real train runs. It is typically expected that these results will be within 5–10% accuracy of the recorded data. However, such a large margin could allow errors in the programming to be overlooked, resulting in an inaccurate model. This paper presents a method for error checking and validating the kinematics of train simulators based on comparison with calculated results, which are found by solving the fundamental equations governing train motion. A typical train run comprises of a combination of two or more of the four stages: accelerating, cruising, coasting and braking. Each stage is considered as a separate scenario for which the equations must be solved, in order to find the running time, distance travelled and energy consumption of the vehicle. This validation method is applied to two train movement simulators currently used for research. Certain specific scenarios for which analytical solutions are available are run in each simulator. The differences from the analytical solution in each test case are quantified, allowing the simulators to be compared to each other and the exact solution.

OPTIMISING ENERGY SAVING IN METRO SYSTEMS THROUGH CHARACTERISTIC EVALUATION

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Abstract

As it expands, the rail industry is concerned not only with maintaining service quality and managing increased demand, but with improving energy efficiency. Whilst it is important that future passenger infrastructures, rolling stock and operations are designed sustainably, existing systems need to reduce their environmental impacts to meet international efficiency targets. A number of energy-saving solutions have been developed to achieve this, often showing excellent results in simulation and for selected case studies. However, operators face a difficult decision when choosing solutions to implement, as these results give limited information on transferability. It may be obvious that a particular solution is more suited for high speed rail than a metro, given the differences between these systems. Yet it could just as easily be the case that a solution which works for one metro is not effective for another, due to certain factors. Through the application of a previously developed method, these factors are investigated for different metro systems. The impact of route, vehicle and service characteristics on the application of energy saving solutions is evaluated, allowing the characteristics with greatest influence to be determined. From this information, recommendations are made as to which solutions are most appropriate for the different systems investigated.

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Investigation into Train Positioning Systems for Saving Energy with Optimised Train Trajectories

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Abstract— One approach to reduce energy consumption in railway systems is to implement optimised train trajectories. These are speed profiles that reduce energy consumption without foregoing customer comfort or running times. This is achieved by avoiding unnecessary braking and running at reduced speed whilst maintaining planned arrival times. An optimised train trajectory can be realised using a driver advisory system (DAS). The optimal train trajectory approach needs a variety of input data, such as the train's position, speed, direction, gradient, maximum speed, dwell time, and station locations. Many studies assume the availability of a very accurate train position in real time. However, providing and using high precision positioning data is not always the most cost-effective solution. The aim of this research is to investigate the use of appropriate positioning systems, with regard to their performance and cost specifications, with optimised trajectories. This paper first presents a single train trajectory optimisation to minimise overall energy consumption. It then explores how errors in train position data affect the total consumed energy, with regard to the tractive force due to gradient when following the optimised trajectory. A genetic algorithm is used to optimise the train speed profile. The results from simulation indicate that a basic GPS system for specifying train position is sufficient to save energy via an optimised train trajectory. The authors investigate the effect of error in positioning data, to guarantee the reliability of employing the optimised solution for saving energy whilst maintaining an acceptable journey time.

Keywords— DAS; Optimised Train Trajectories; Energy Saving; Train Positioning System

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BACK   ◆◆◆   CLOSE WINDOW

Appendix C: Fisher's Iris Dataset

Iris Setosa				Iris Veriscolor				Iris Virginica			
Sepal Length	Sepal Width	Petal Length	Petal Width	Sepal Length	Sepal Width	Petal Length	Petal Width	Sepal Length	Sepal Width	Petal Length	Petal Width
5.1	3.5	1.4	0.2	7	3.2	4.7	1.4	6.3	3.3	6	2.5
4.9	3	1.4	0.2	6.4	3.2	4.5	1.5	5.8	2.7	5.1	1.9
4.7	3.2	1.3	0.2	6.9	3.1	4.9	1.5	7.1	3	5.9	2.1
4.6	3.1	1.5	0.2	5.5	2.3	4	1.3	6.3	2.9	5.6	1.8
5	3.6	1.4	0.2	6.5	2.8	4.6	1.5	6.5	3	5.8	2.2
5.4	3.9	1.7	0.4	5.7	2.8	4.5	1.3	7.6	3	6.6	2.1
4.6	3.4	1.4	0.3	6.3	3.3	4.7	1.6	4.9	2.5	4.5	1.7
5	3.4	1.5	0.2	4.9	2.4	3.3	1	7.3	2.9	6.3	1.8
4.4	2.9	1.4	0.2	6.6	2.9	4.6	1.3	6.7	2.5	5.8	1.8
4.9	3.1	1.5	0.1	5.2	2.7	3.9	1.4	7.2	3.6	6.1	2.5
5.4	3.7	1.5	0.2	5	2	3.5	1	6.5	3.2	5.1	2
4.8	3.4	1.6	0.2	5.9	3	4.2	1.5	6.4	2.7	5.3	1.9
4.8	3	1.4	0.1	6	2.2	4	1	6.8	3	5.5	2.1
4.3	3	1.1	0.1	6.1	2.9	4.7	1.4	5.7	2.5	5	2
5.8	4	1.2	0.2	5.6	2.9	3.6	1.3	5.8	2.8	5.1	2.4
5.7	4.4	1.5	0.4	6.7	3.1	4.4	1.4	6.4	3.2	5.3	2.3
5.4	3.9	1.3	0.4	5.6	3	4.5	1.5	6.5	3	5.5	1.8
5.1	3.5	1.4	0.3	5.8	2.7	4.1	1	7.7	3.8	6.7	2.2
5.7	3.8	1.7	0.3	6.2	2.2	4.5	1.5	7.7	2.6	6.9	2.3
5.1	3.8	1.5	0.3	5.6	2.5	3.9	1.1	6	2.2	5	1.5
5.4	3.4	1.7	0.2	5.9	3.2	4.8	1.8	6.9	3.2	5.7	2.3
5.1	3.7	1.5	0.4	6.1	2.8	4	1.3	5.6	2.8	4.9	2
4.6	3.6	1	0.2	6.3	2.5	4.9	1.5	7.7	2.8	6.7	2
5.1	3.3	1.7	0.5	6.1	2.8	4.7	1.2	6.3	2.7	4.9	1.8
4.8	3.4	1.9	0.2	6.4	2.9	4.3	1.3	6.7	3.3	5.7	2.1
5	3	1.6	0.2	6.6	3	4.4	1.4	7.2	3.2	6	1.8
5	3.4	1.6	0.4	6.8	2.8	4.8	1.4	6.2	2.8	4.8	1.8
5.2	3.5	1.5	0.2	6.7	3	5	1.7	6.1	3	4.9	1.8
5.2	3.4	1.4	0.2	6	2.9	4.5	1.5	6.4	2.8	5.6	2.1
4.7	3.2	1.6	0.2	5.7	2.6	3.5	1	7.2	3	5.8	1.6
4.8	3.1	1.6	0.2	5.5	2.4	3.8	1.1	7.4	2.8	6.1	1.9
5.4	3.4	1.5	0.4	5.5	2.4	3.7	1	7.9	3.8	6.4	2
5.2	4.1	1.5	0.1	5.8	2.7	3.9	1.2	6.4	2.8	5.6	2.2
5.5	4.2	1.4	0.2	6	2.7	5.1	1.6	6.3	2.8	5.1	1.5
4.9	3.1	1.5	0.2	5.4	3	4.5	1.5	6.1	2.6	5.6	1.4
5	3.2	1.2	0.2	6	3.4	4.5	1.6	7.7	3	6.1	2.3
5.5	3.5	1.3	0.2	6.7	3.1	4.7	1.5	6.3	3.4	5.6	2.4
4.9	3.6	1.4	0.1	6.3	2.3	4.4	1.3	6.4	3.1	5.5	1.8
4.4	3	1.3	0.2	5.6	3	4.1	1.3	6	3	4.8	1.8
5.1	3.4	1.5	0.2	5.5	2.5	4	1.3	6.9	3.1	5.4	2.1
5	3.5	1.3	0.3	5.5	2.6	4.4	1.2	6.7	3.1	5.6	2.4
4.5	2.3	1.3	0.3	6.1	3	4.6	1.4	6.9	3.1	5.1	2.3
4.4	3.2	1.3	0.2	5.8	2.6	4	1.2	5.8	2.7	5.1	1.9
5	3.5	1.6	0.6	5	2.3	3.3	1	6.8	3.2	5.9	2.3
5.1	3.8	1.9	0.4	5.6	2.7	4.2	1.3	6.7	3.3	5.7	2.5
4.8	3	1.4	0.3	5.7	3	4.2	1.2	6.7	3	5.2	2.3
5.1	3.8	1.6	0.2	5.7	2.9	4.2	1.3	6.3	2.5	5	1.9
4.6	3.2	1.4	0.2	6.2	2.9	4.3	1.3	6.5	3	5.2	2
5.3	3.7	1.5	0.2	5.1	2.5	3	1.1	6.2	3.4	5.4	2.3
5	3.3	1.4	0.2	5.7	2.8	4.1	1.3	5.9	3	5.1	1.8

Appendix D: Subsystem Results Graphs

Urban Commuter

### *PCA Analysis Results: Gradient = 10m/km*
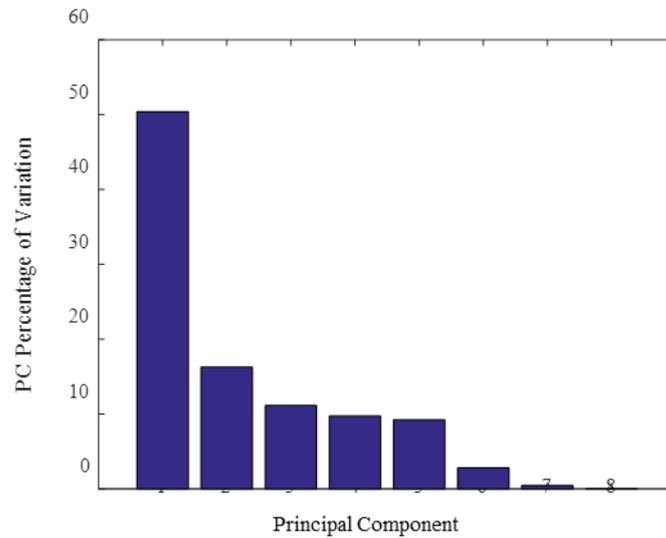
Figure 79: Percentage contribution of each PC to the total variation of the UComm subsystem gradient dataset

Table 37: PC scores for UComm subsystem with a gradient of 10m/km

	PC1	PC2	PC3	PC4
Efficiency	-0.2	**0.5** (0.4)	**0.6** (0.7)	**0.5** (0.4)
Mass	-0.2	0.5	**-0.6** (-0.5)	0.3 (0.4)
Aerodynamics	-0.2	0.4	**0.1** (0.0)	-0.8
Maximum Speed	-0.4	**-0.2** (-0.3)	0.1	**-0.1** (0.0)
Regeneration Use	-0.2	0.4	**0.0** (0.1)	-0.3 (-0.1)
Coasting Limit	-0.5	-0.1	0.0	0.0
Energy	-0.5	-0.1	-0.4	0.1
Journey Time	0.4	0.3	-0.2	**0.1** (0.0)
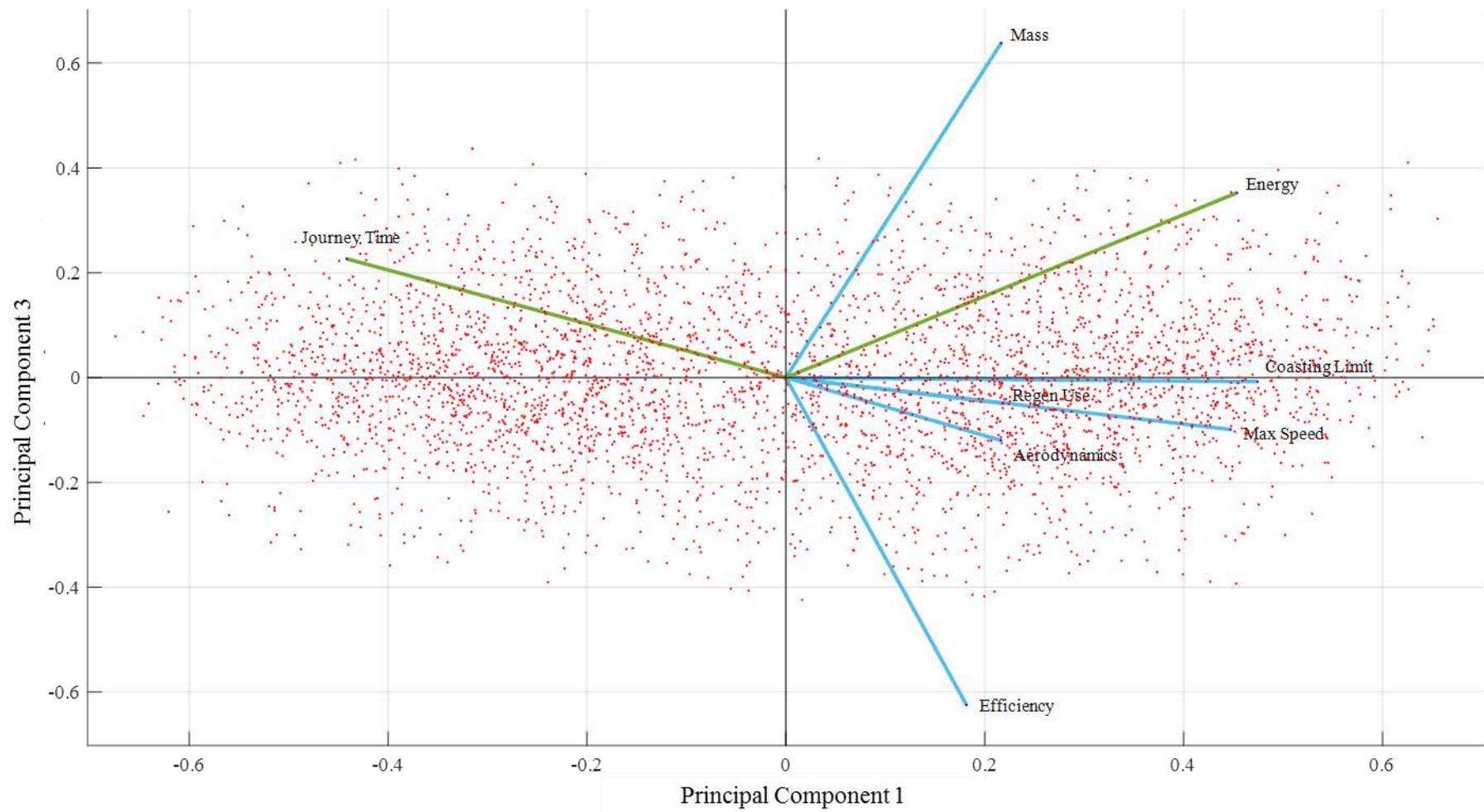
Figure 80: Bi-plot of PC1 and PC3 for the UComm gradient dataset
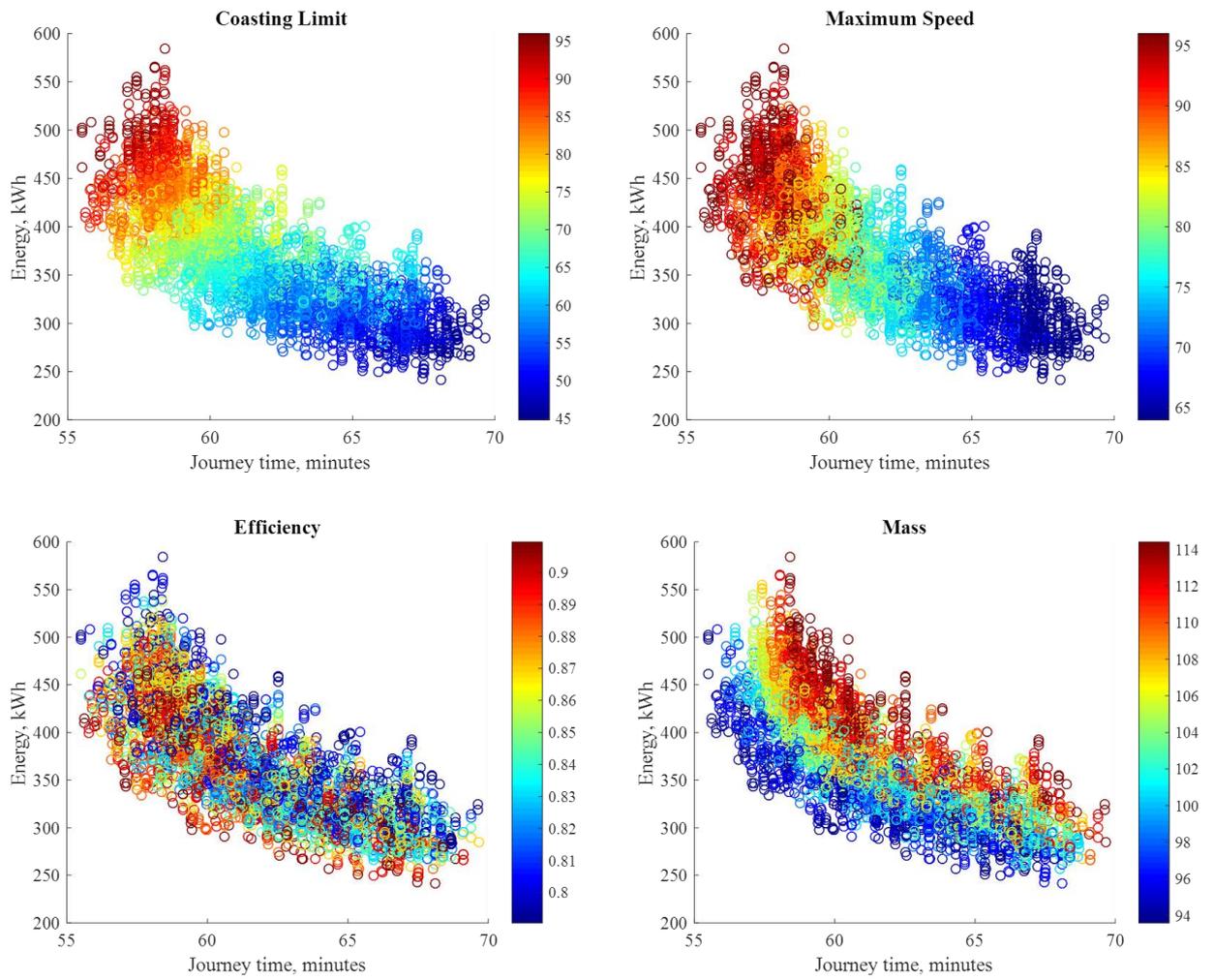
Figure 81: TIPs highlighting the relationships each of the four key factors have with energy and journey time, for the UComm gradient dataset

Inter-City Commuter

PCA Analysis Results: Gradient = 10m/km
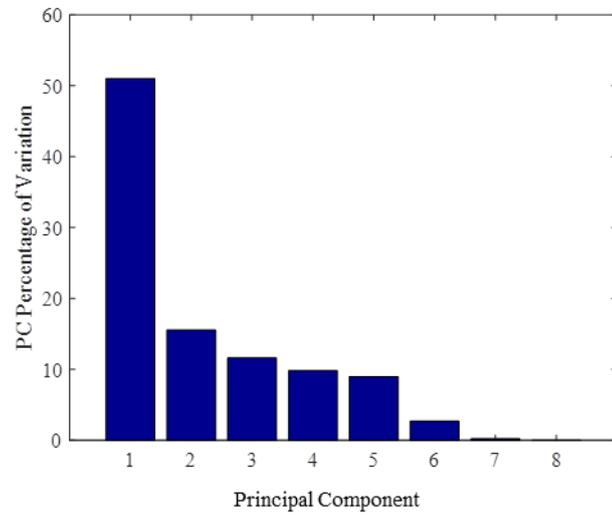
Figure 82: : Percentage contribution of each PC to the total variation of the ICComm subsystem gradient dataset
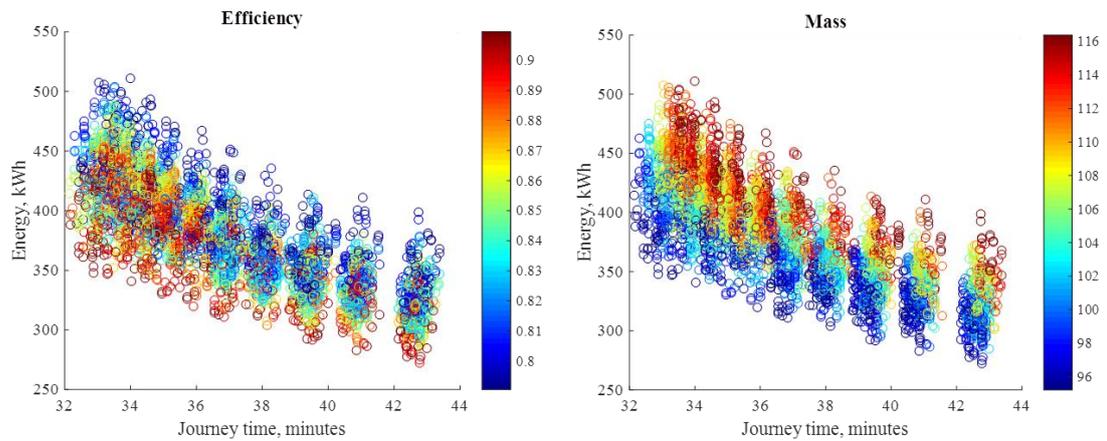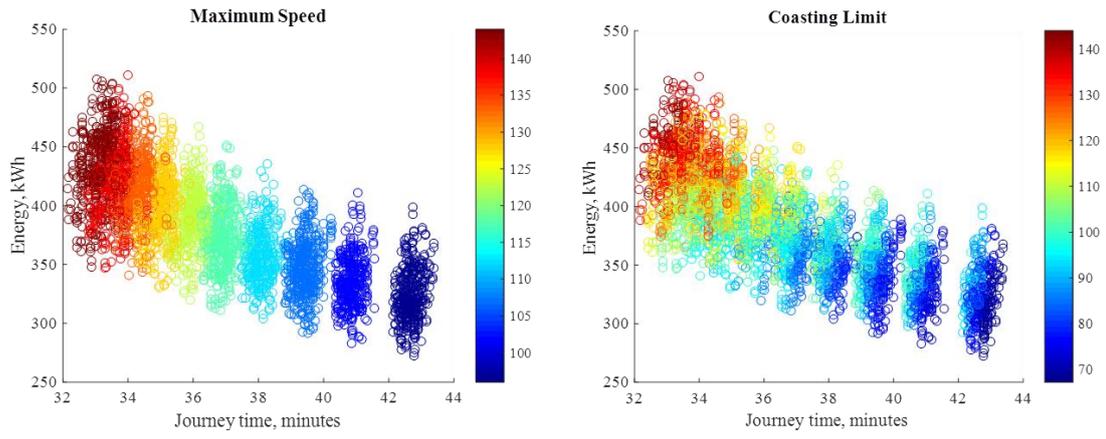
Figure 83: TIPs highlighting the relationships each of the four key factors have with energy and journey time, for the ICComm gradient dataset
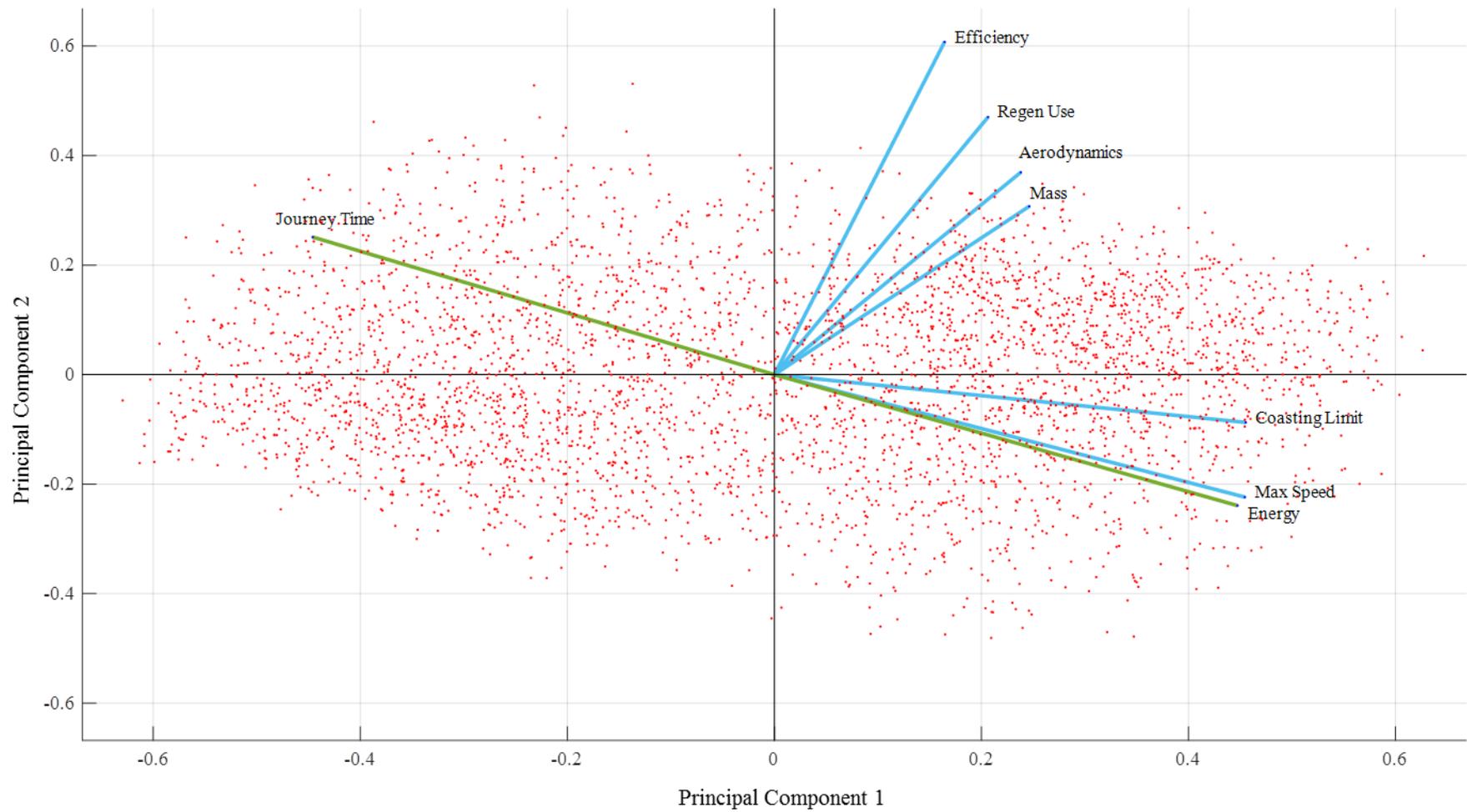
Figure 84: Bi-plot of PC1 and PC2 for the ICComm gradient dataset

## High Speed Commuter

PCA Analysis Results: Interstation distance =35km
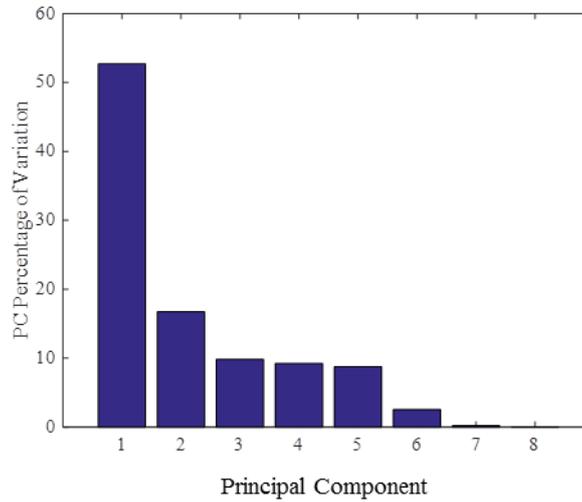
Figure 85: Percentage contribution of each PC to the total variation of the HSComm subsystem interstation distance dataset

Table 38: PC scores for the High Speed Commuter subsystem with interstation distance = 35km

|	PC1	PC2	PC3	PC4
Efficiency	-0.2	0.6	0.1	0.1
Mass	-0.2	0.4	-0.7	0.5
Aerodynamics	-0.2	0.4	0.7	0.3
Maximum Speed	**-0.5** (-0.4)	-0.2	0.0	0.0
Regeneration Use	-0.2	0.4	-0.2	-0.8
Coasting Limit	-0.5	-0.1	0.0	0.0
Energy	-0.5	-0.2	0.0	0.1
Journey Time	0.5	0.2	0.0	0.0
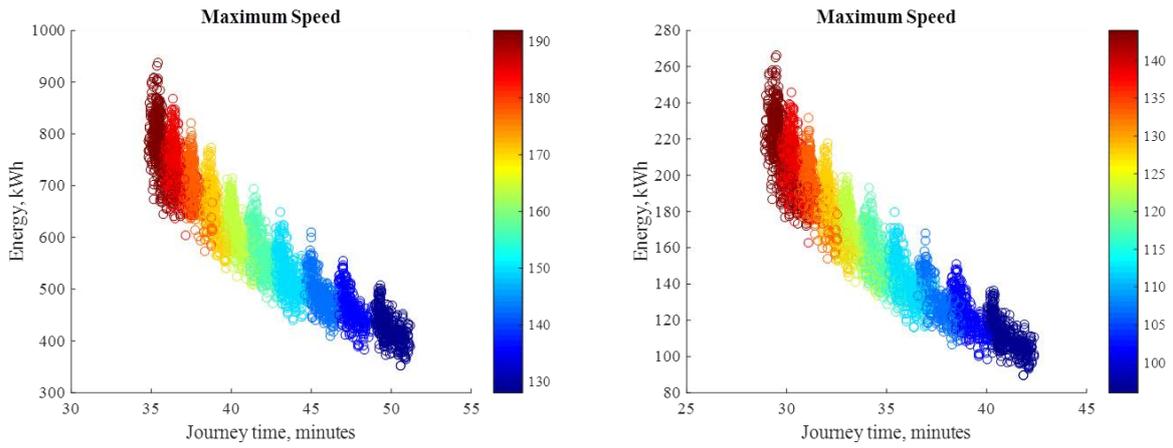
Figure 86: Comparison of the maximum speed scatter plots for HSComm (left) and ICComm (right) subsystems
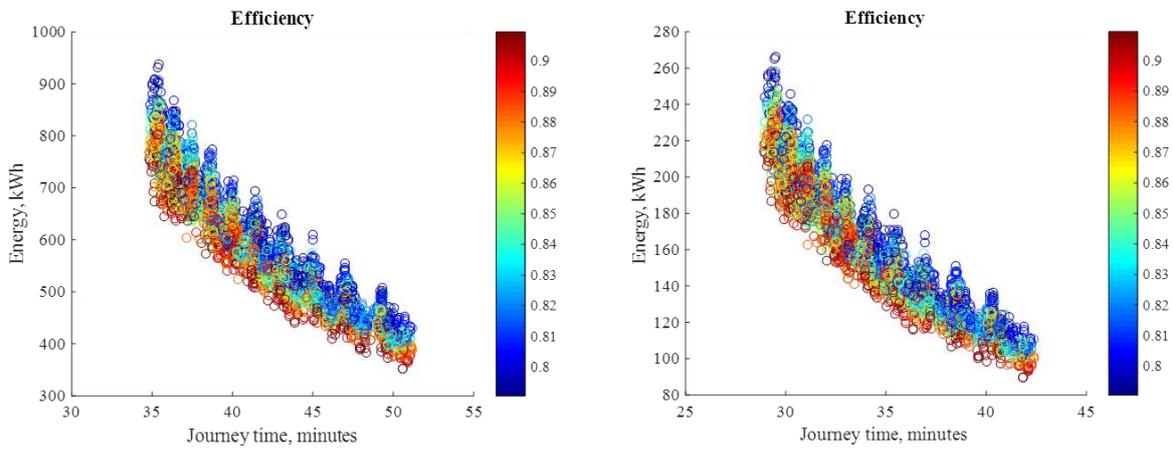

**Figure 87: Comparison of the efficiency scatter plots for HSComm (left) and ICComm (right) subsystems**
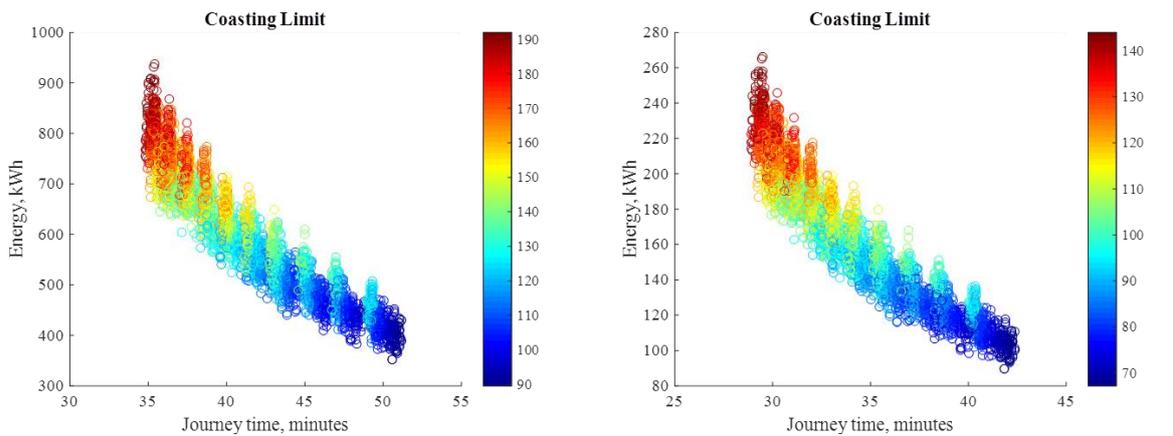
Figure 88: Comparison of the coasting limit scatter plots for HSComm (left) and ICComm (right) subsystems

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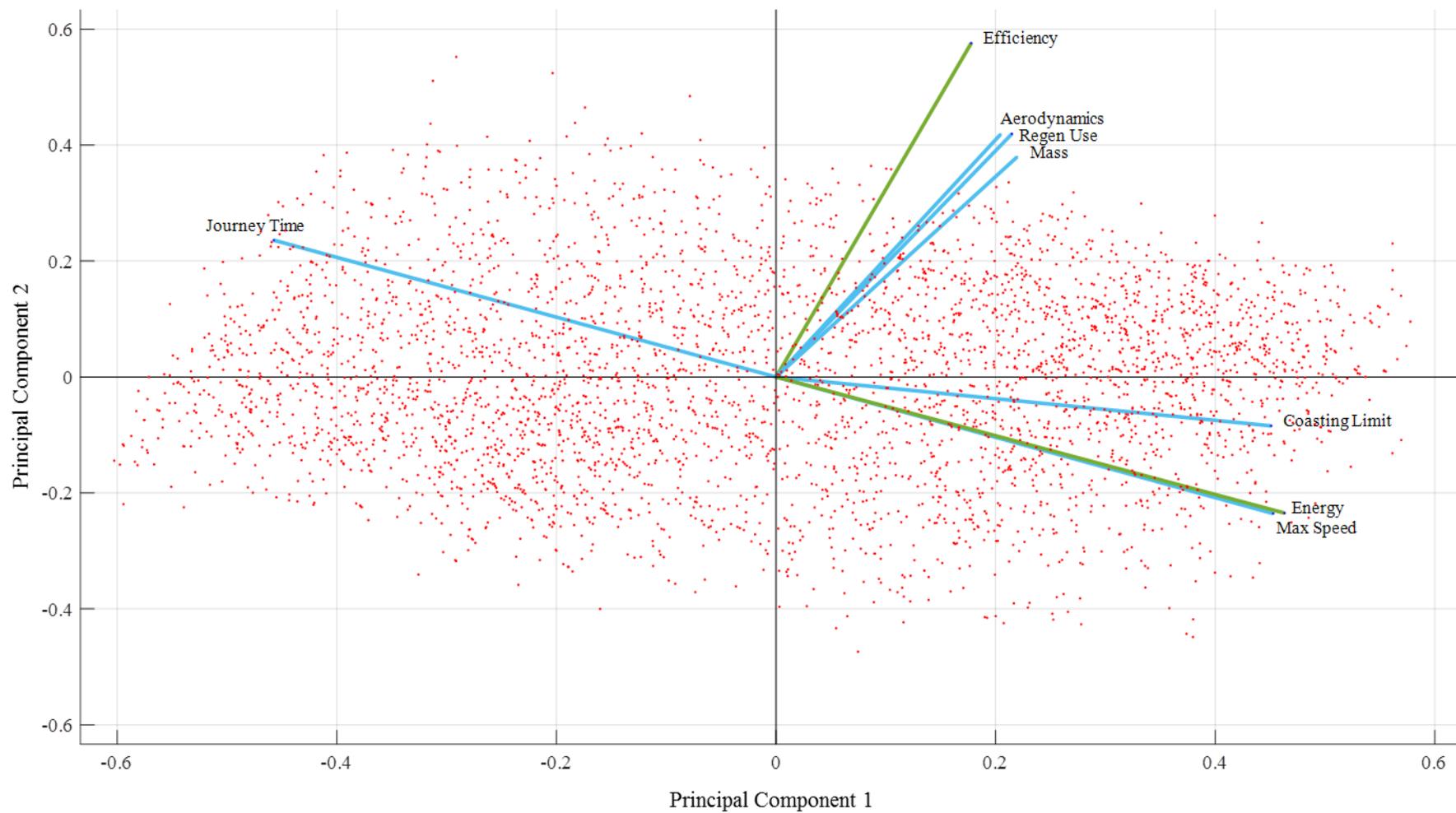
Figure 89: Bi-plot of PC1 and PC2 for the HSComm maximum interstation distance = 35km dataset

## PCA Analysis Results: Gradient = 10m/km
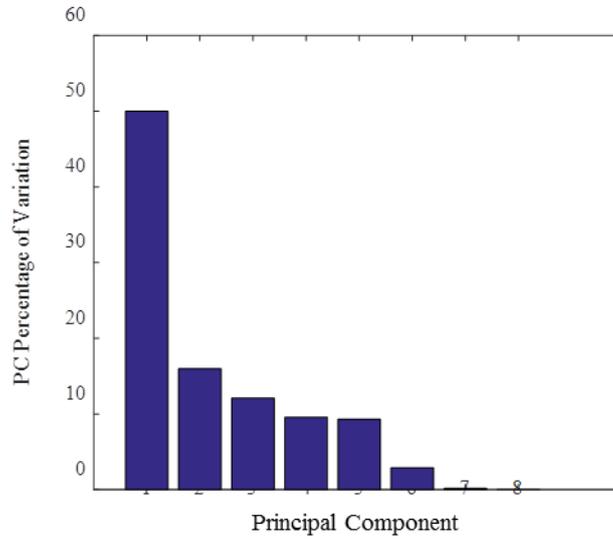
Figure 90: Percentage contribution of each PC to the total variation of the HSComm subsystem uphill gradient dataset

Table 39: PC scores for HSComm subsystem with a gradient of 10m/km

|	PC1	PC2	PC3	PC4
Efficiency	-0.2	**0.7** (0.6)	**-0.4 (-0.5)**	**0.5 (-0.4)**
Mass	**-0.3** (-0.2)	**0.2** (0.3)	0.7	**0.5 (-0.4)**
Aerodynamics	-0.2	0.4	**0.1** (0.2)	**-0.3 (0.5)**
Maximum Speed	-0.5	-0.2	**-0.3** (-0.2)	**0.0** (-0.1)
Regeneration Use	-0.2	**0.4** (0.5)	**0.2** (-0.1)	**-0.7 (0.5)**
Coasting Limit	**-0.4** (-0.5)	**0.0** (-0.1)	**-0.2** (-0.1)	0.0
Energy	-0.4	**-0.3** (-0.2)	0.3	**0.0**
Journey Time	**0.5** (0.4)	**0.2** (0.3)	0.3	0.0

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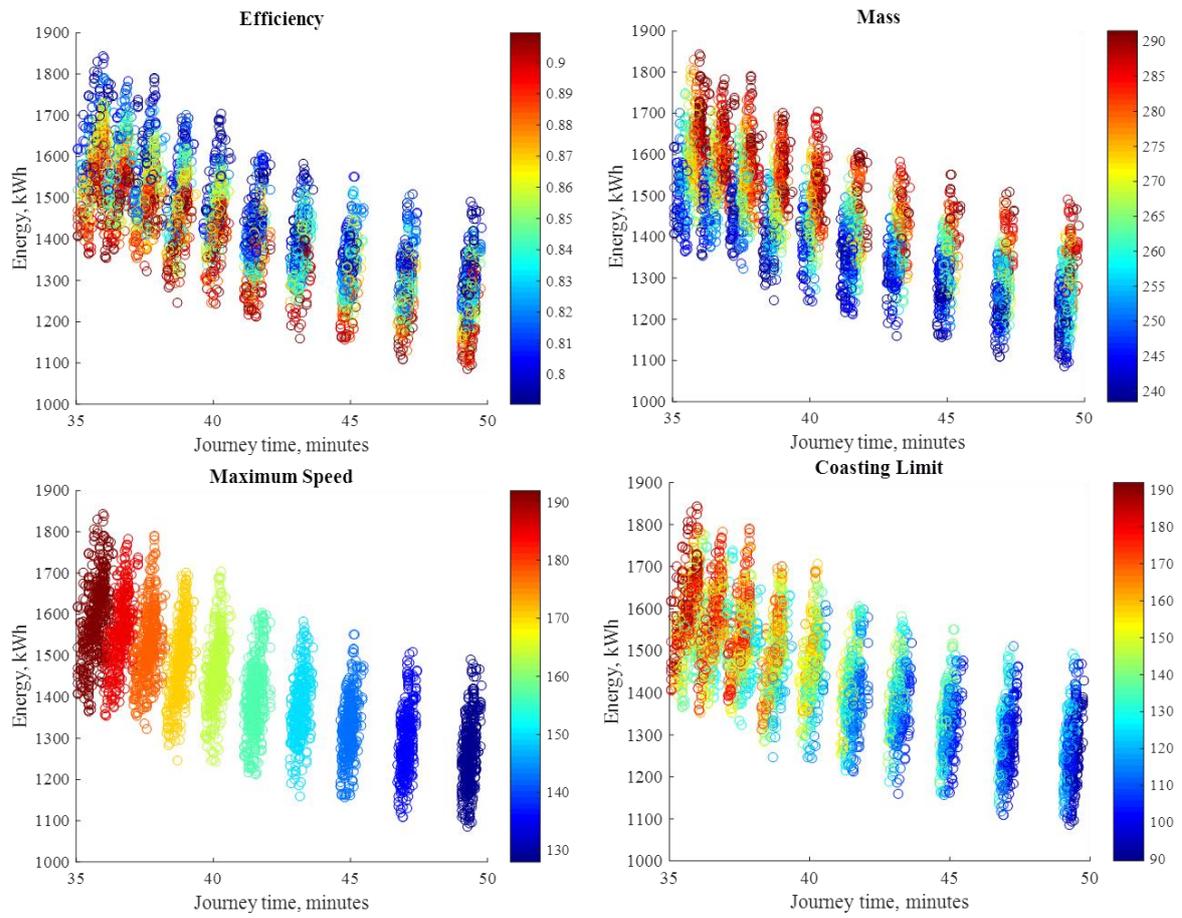
Figure 91: TIPs highlighting the relationships each of the four key factors have with energy and journey time, for the HSComm gradient dataset
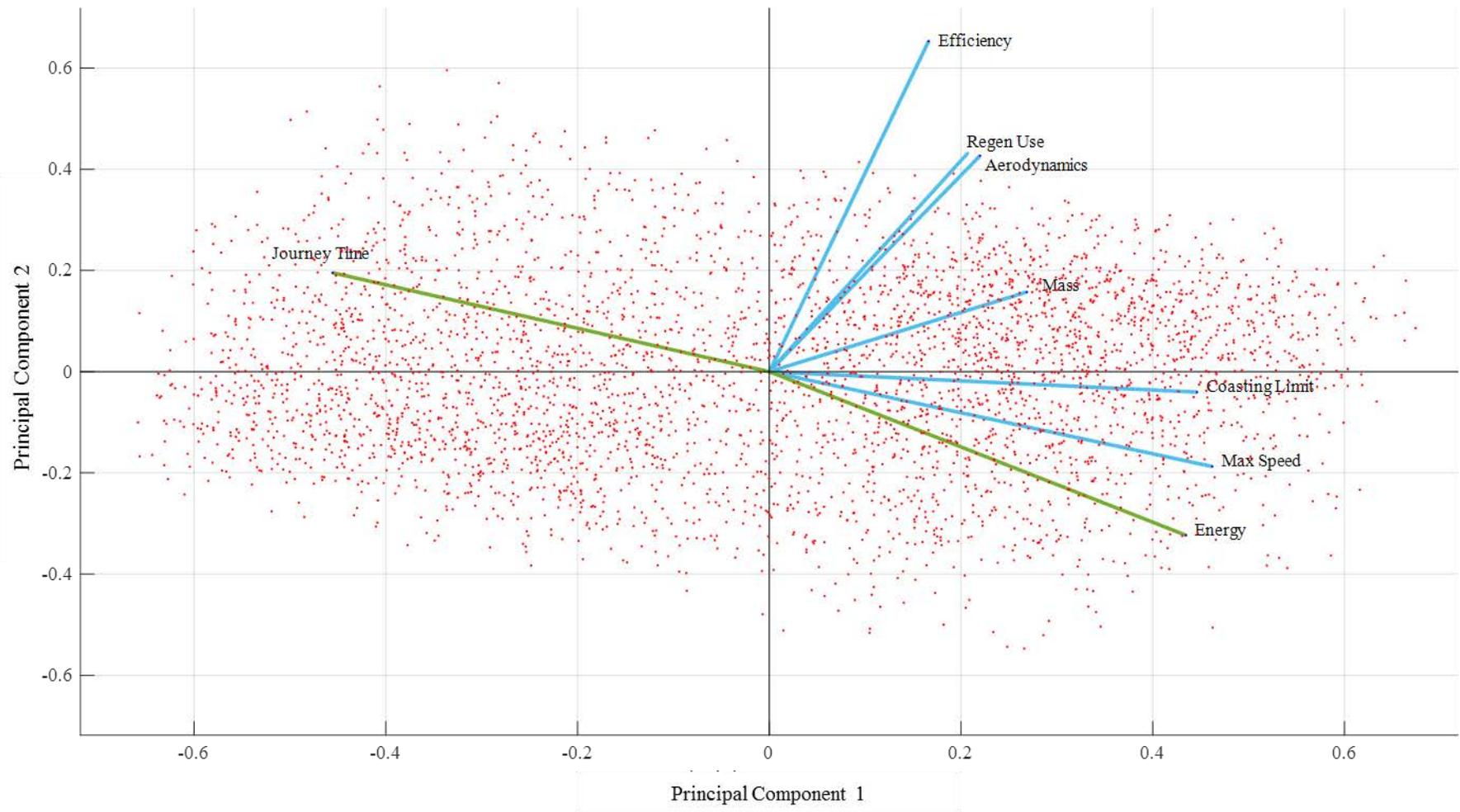
Figure 92: Bi-plot of PC1 and PC2 for the HSComm gradient dataset

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Appendix E: Summary of Personal Communications

I approached Mr Neubauer via email with an initial draft of Figure 71 (Ratios for the TE and BE curves for PMSMs and IMs) and he advised me on the appropriateness of the numbers given. Based on his recommendations, the values for the torque and power curves were changed. He also explained the significant impact the thermal environment can have on motor performance and the difficulty in obtaining this information: the thermal environment and ventilation is therefore assumed to be the same for the two motors. In a further exchange, Dr Neubauer provided a rough estimate of the prices for rail traction motors depending on their application, although he stressed that this was an estimate, and that the price may vary depending on the contract and design issues.