Determining the role of hydrogen in the future UK's private vehicle fleet using growth and Lotka-Volterra concepts.

Faculty of Computing, Engineering, and the Built Environment

School of Engineering and Built Environment

Student: Sahdia Maryam

Student Number: 08448432

Submission Date: March 2021

Director of Studies: Dr. Florimond Gueniat

Second Supervisors: Dr. Roshni Paul

A thesis submitted to Birmingham City University in partial fulfilment of the requirements for the degree of Doctor of Philosophy

Declaration

I declare that this thesis has been composed solely by myself and that it has not been submitted, in whole or in part, in any previous application for a degree. Except where states otherwise by reference or acknowledgement, the work presented is entirely my own.

Name: Sahdia Maryam
Date: 01/03/2021

Acknowledgements

I am sincerely grateful to Allah Almighty for giving me the strength, patience, and most importantly, persistence to undertake and complete this PhD journey. I further extend my gratitude to my parents, brothers, and sisters whose patience, and unwavering support has kept me on this path and made this journey possible. To my husband, Magdy, and my children, Aisha, Zainab, Yusuf, and Ibrahim – thank you for putting up with me during parts of this journey. I would also like to express my sincere gratitude to my supervisory team, especially Dr. Florimond Gueniet whose contribution motivated the completion of this thesis when it was easier to walk away, and Dr. Roshni Paul for her encouragement and help that enabled the completion of this project. The encouragement and support I received from Dr. Adrian Cole, Dr. Manjit Srai, Dr. Dimitra Kalaitzi, and the late Dr. Christine E. Lloyd for supervising the earlier and middle stages of my PhD. I am particularly grateful for being given the opportunity to undertake this PhD by Birmingham City University.

Abstract

This research aimed to explore effective strategies for the UK's private vehicle fleet to transition to a hydrogen one. The main barrier for hydrogen is the lack of refuelling infrastructure impacting the uptake of hydrogen-based vehicles. Current studies focus on the introduction of hydrogen alone with a pre-determined supply chain or consider the study of one part of the supply chain such as the storage. A computational modelling approach was considered to reflect the private vehicle market based on predator-prey concepts. The Lotka-Volterra model captures the dynamic behaviour between two or more competing species/technologies to simulate the introduction of alternative vehicle types and their impact on current vehicles. The behaviour of the predator-prey model was limited to reflect the private vehicle fleet by developing a first-order growth model representing the growth of conventional vehicles over the last 50 years. By modelling the growth of conventional vehicles, the private vehicle fleet was considered holistically rather than a selected supply chain(s). The implication of this was to overcome the issue of lack of data and insights to forecasting hydrogen and alternative fuels, whilst capturing the mutually interaction between multiple competing vehicle types. A key finding associated with this thesis was the demonstration that the modified Lotka-Volterra model is suitable to represent the dynamic relationship of introducing new and multiple vehicle types into the current private vehicle fleet. The results indicated that the model simplified the current hydrogen infrastructure problem by reducing the number of factors and variables considered, offering a robust alternative modelling tool. This thesis suggests that it is unlikely that the entire private fleet will be displaced by hydrogen vehicles, and the upper limit should be set at 50% of the market. The optimum strategy for the UK is 80:20 in favour of non-fuel cell hybrids and electric vehicles to hydrogen-based ones focusing on a centralised network of stations. It is recommended that the HRS is at least operated at 75% increasing to maximum when necessary, avoiding under-utilisation. The main implications are that stakeholders can plan according to the best-scenario from a holistic view to shape the future of UK's private fleet.

Journal Publications

Maryam, S. (2017) Review of modelling approaches used in the HSC context for the UK. *International Journal of Hydrogen Energy*, 42 (39): 24927–24938. doi:10.1016/j.ijhydene.2017.04.303.

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List of Symbols

Symbol	**Definition**
$\dot{m}_t$	Total mass of fuel consumed by the fleet in a year including the mass wasted.
$\dot{m}_w$	Mass being wasted
m	This is the total mass of a fuel type used per year e.g. the total mass of petrol, or hydrogen etc.
N_v	Number of vehicles
m_i	Mass of the fuel consumed per vehicle per year
µ	This is the mass of fuel used annually divided by the mass of fuel consumed by a vehicle.
α	This is the growth rate of a vehicle type or the fleet.
x_1	Number of Internal combustion engine vehicles assuming the role of prey
x_2	Number of Non-fuel cell & electric vehicles (Predator 1)
x_3	Number of hydrogen-based vehicles (Predator 2)
a, d, g	Growth rates of vehicle types i.e. rate of increase per unit time
b	The coefficient of predation rate (attack rate of predator 1 on prey)
c	Efficiency of predator 1
e	The attack rate of predator 2 on prey
f	Attack rate of predator 1 on predator 2
h	Hydrogen efficiency
i	Conversion efficiency of NFC-EVs
μ_1	Total fuel input for prey
μ_2	Total fuel input for predator 1
μ_2	Total fuel input for predator 2

Nomenclature

Abbreviation	**Definition**
AFV	Alternative Fuel Vehicles
CCS	Carbon Capture and Storage
EVs	Electric Vehicles
FCs	Fuel Cells
HBVs	Hydrogen-based Vehicles
HCs	Hydrocarbons
HFCVs	Hydrogen Fuel Cell Vehicles
HFC-REs	Hydrogen Fuel Cell Range Extenders
HRS	Hydrogen Refuelling Station
HSCs	Hydrogen Supply Chains
ICEVs	Internal combustion Vehicles
LVM	Lotka-Volterra Model
NGVs	Natural Gas Vehicles
NRES	Non-Renewable Energy Sources
PEMFC	Proton Exchange Membrane FC
PES	Primary Energy Sources
RES	Renewable Energy Sources
SCs	Supply Chains
SES	Secondary Energy Sources
SMR	Steam Methane Reforming
WE	Water Electrolysis

I dedicate this thesis to women.
Mothers, daughters, and sisters.
Whoever and wherever you are,
keep believing and fighting for a better,
fairer, and safer tomorrow
from the ashes of today’s struggle.

Chapter 1: Introduction

1.1 Overview of the chapter

This chapter introduces the proposal for research presented in this thesis. It will further discuss the motivation behind the study concerning the role hydrogen will play as a transportation fuel for the private passenger vehicle fleet. Currently, the private vehicle sector relies on conventional fuel-based vehicles such as petrol and diesel. Conventional fuel contributes significantly to the number of emissions projected into the environment alongside the usage of finite resources. This thesis considers alternative fuel-based vehicles focusing on hydrogen fuel cell vehicles, the environmental implications alongside the competitiveness of hydrogen as a transport fuel. The chapter commences with a section on the background of the research area, followed by the rationale, research aims and objectives, and an overview of the thesis chapters. The research background provides an overview of the complexity of introducing a new fuel for passenger vehicles and the corresponding infrastructure.

1.2 Background

Research and development for alternative transport fuels (ATFs) are mainly driven by the environmental implications of conventional fuels (Baufumé et al., 2013a; Yang and Ogden, 2013; Yoon et al., 2022). Some key drivers include air and noise pollution (Hitchcock et al., 2014; Sharma and Ghoshal, 2015); harmful health issues related to pollution such as inflammation of airways, reducing lung function, and asthma (Hitchcock et al., 2014; AA, 2017); energy security and the consumption of finite resources (Wickham et al., 2022); regulations and government policies (European Commission, 2016; GOV.UK, 2017a); growth of global energy demand due to rising population and living standards (Dincer and Acar, 2015; Babar et al., 2021).

In order to assess and mitigate climate change, a renewed effort has been made to diversify energy feedstock (resources consumed to produce energy) and supply, especially for the transportation sector (Yang and Ogden, 2013); whether carbon capture and storage (CCS) plays an intermediary solution (Baufumé et al., 2013a; CCS, 2017). Primary energy sources (PES) are found in the natural environment. They can be used directly, e.g., coal, oil, gas, biofuels. Whereas secondary energy sources (SES), such as hydrogen and electricity, are formed using PES (Wietschel et al., 2006; Ajanovic and Haas, 2021). The diversification of feedstock can pose a problem for passenger vehicles to use directly, e.g., the engine needs to be modified for different blends of fuel. Hydrogen and electricity overcome this issue by converting different feedstock into either one. These are then used to fuel a hydrogen-based vehicle (HBV) or an electric vehicle (EV). So, converting these various primary fuels into hydrogen enables the diverse geographically dominant fuels to become an international fuel. There is interest internationally to develop the current and new hydrogen technologies to provide cleaner and greener alternative options to increase energy security concerns alongside economic considerations (Holladay et al., 2009). It is also likely that both hydrogen and electricity will be used as tertiary fuels in the future. As energy carriers, hydrogen and electricity supplement each other, e.g. hydrogen is used for energy storage and converted to electricity when required to provide an appropriate long-term solution to reduce $C0_2$ emissions (Dincer and Acar, 2015; Weger et al., 2021).

1.2.1 The characteristics of hydrogen

Hydrogen is the first element in the periodic table. It is a carbon-free, colour-less, odourless, non-toxic gas and has high specific energy based on mass (Momirlan and Veziroglu, 2005; Kovač et al., 2021). The advantage of hydrogen is that it is the most abundant element in the universe found in all organic matter (Dincer and Acar, 2015). Hydrogen is not considered a GHG, while its secondary impact on the GHG effect due to leakage is negligible as it diffuses with air straight away without polluting the ground or groundwater (Air Products, 2017; Kovač et al., 2021). However, hydrogen is never found in its pure form naturally but must be separated from another substance requiring energy input (Tolga Balta et al., 2009). This makes hydrogen a secondary energy source, just like electricity, often known as a vector or an energy carrier (Mazloomi and Gomes, 2012; Ajanovic and Haas, 2021) at the foundation of a carbon-neutral system of energy production and usage.

1.2.2 Challenges for hydrogen as a transport fuel

Overcoming the challenges that hydrogen faces to become a dominant transportation fuel for passenger vehicles offers many advantages over current fossil-based fuels. However, as with introducing any new technology, hydrogen also poses several issues. From the literature, the most commonly cited technological barriers are the high purchase price of hydrogen fuel cell vehicles (HFCVs) and the lack of hydrogen refuelling infrastructure (Hardman et al., 2017a; Ratnakar et al., 2021). The high cost of HFCVs has mainly attributed to the cost of fuel cells (FCs), hydrogen storage tanks due to hydrogen being a gas at room temperature and hydrogen plant components, which are higher in cost than their conventional counterparts (Hardman et al., 2017a). An element of cost is also attributed to a lack of economies of scale (Engelen et al., 2016; Seo et al., 2020) and specialised materials in their construction. In terms of hydrogen production, converting other fuels into hydrogen is a costly process, and a considerable amount of electricity is also consumed to produce hydrogen. An alternative is to use the electricity to fuel passenger vehicles than to lose it in the process. So, while hydrogen produced from renewable energy is attractive, it will compete with the same green energy used to extract it. Hydrogen will only be adopted as a dominant fuel if there is a readily available infrastructure to fuel HBVs, cost reduction of cars, and ensuring stable policy framework conditions that support emerging technologies, alongside reduction in risk for long-term investments (Ajanovic and Haas, 2021). An advantage of hydrogen is the potential to decarbonise supply chains because the carbon emissions that are affluent with fossil fuels are not generated when hydrogen is utilised for energy. Both non-carbon emitting energy feedstock and non-carbon energy carriers are required to move away from the carbon-based energy system. The main aim is to have green hydrogen produced via water electrolysis (WE) for a carbon neutral society and in the intermittent period to utilise grey hydrogen (i.e. produced via fossil fuels) (Kovač et al., 2021). While there are many non-carbon feedstocks, e.g., sunlight, wind, hydraulic power, there are only two carbon-neutral energy vectors/carriers, i.e., hydrogen and electricity. Electricity and hydrogen share many synergies in an equivalent way to currency. Electricity is useful for transferring energy over short distances without transferring mass, and hydrogen is advantageous for transferring energy over long distances and storing surplus electricity for peak times. Electricity can transmit, process, and store information, and hydrogen cannot (Scott, 2004). Furthermore, the number of potential feedstock for manufacturing hydrogen – both renewable energy sources (RES) and non-renewable energy sources (NRES), consequently reduces the over-reliance on petroleum products and mitigating GHG emissions. (Momirlan and Veziroglu, 2005; Dodds and McDowall, 2012).

1.2.3 Comparison to other existing fuels

In this section, the properties of hydrogen are compared with other typical transportation fuels in terms of the energy extracted by undergoing combustion (see table 1.1). Petrol and diesel vehicles have dominated the market mainly for the last 100 years. Natural gas vehicles (NGVs) currently constitute just below 26.5 million vehicles, with 31,246 NG refuelling stations worldwide (NGV Global, 2019).

The amount of energy released from a fuel that undergoes complete combustion is often specified as higher or lower heating values (HHV/LHV). The difference is that the HHV represents the entire heat produced while the LHV excludes any heat consumed to vaporise water during combustion (Dodds and McDowall, 2012). The mass-specific LHV of H_2 is almost three times as high as either petrol, diesel, or NG. While the energy density is a clear advantage, the volumetric energy content provides a challenge for storage, e.g. a 15 gallon tank of gasoline will house 90lbs of gasoline compared to a 60 gallon vessel of hydrogen that stores 34lbs of hydrogen (Sharma and Ghoshal, 2015). Hydrogen is usually compressed and stored at high pressures to store enough quantities. In terms of energy yield, hydrogen is 2.75 times greater.

Table 1. 1: Comparison of key properties of hydrogen, NG, petrol, and diesel

	Specific Energy		**Volumetric Energy Density**		**Flammability limits in air**	**Auto-ignition temperature**
	HHV (kWh/kg)	LHV (kWh/kg)	HHV (kWh/L)	LHV (kWh/L)	Vol(%)	°C
Hydrogen H_2	39.4	33.3	0.00354	0.003	4-75	585
Natural gas CH_4	14.5	13.1	0.0109	0.0098	5-15	~ 760
Petrol $C_4 - C_{12}$	13.0/12.89	12.3/12.06	9.6	9.1	1.0-7.6	~ 350
Diesel $C_8 - C_{25}$	12.67	11.83	10.6	9.98	1.0-6	~ 265
1 kWh = 3.6 MJ (Conversion factor used)						

(EngineeringToolbox, 2003; Staffell, 2011; Verhelst et al., 2012; NFPA, 2013; Energy Research Partnership, 2016; Çelebi and Aydın, 2019).

Hydrogen has broad flammability limits ranging from 4.1 to 74.8 Vol-% (of H_2 in air) (Kovač et al., 2021), so hydrogen is compatible with lean-burn operation. Verhelst et al., (2012) made the case that hydrogen, despite challenges, provides the possibility of increasing the power output by more than 15% compared to gasoline engines. Hydrogen's broad range of flammability limits and high flame speeds under lean conditions allow highly efficient lean-burn engine load strategies to lead to higher engine efficiencies. The dual-fuel capacity of the HFC-RE might aid in overcoming the chicken-and-egg problem of developing a hydrogen infrastructure or investing in the implementation of the hydrogen vehicle fleet (Verhelst and Wallner, 2009; Verhelst et al., 2012).

1.3 Rationale

To extenuate the environmental impact of air pollution and GHGs, it is essential that transport displaces conventional finite fuels with renewable and greener alternatives. Hydrogen, an ideal replacement for conventional fuels, is hindered by many technological and, most importantly, infrastructural issues (Hardman et al., 2017a). The need to rapidly build a sustainable hydrogen infrastructure becomes imperative with the increase in demand. However, the current lack of infrastructure dampens the commitment to hydrogen as a transport fuel without policy changes and initiation on behalf of various stakeholders to move to a more sustainable infrastructure (Maryam, 2017).

The future UK's private vehicle fleet must be multi-fuel based to achieve sustainability and fuel security. Therefore, a more comprehensive forecasting models are required to identify the hydrogen space from which the role of different pathways is analysed subject to demand and location dependent factors. So, while there is a need to focus on individual HSC pathways, there is a greater need to identify the role hydrogen will play. Will road vehicles in the UK undergo a total transition to a hydrogen economy, partial transition, or minimal one where only certain fleet types will utilise hydrogen in the future? This research explores how Lotka-Volterra (LV) and growth models can support better hydrogen forecasts for the UK. The primary focus is on the UK because of the government targets and the initiative to achieve the targets (UK Government, 2019). The UK is one of the leading nations in transforming the energy demand of transport and other sections from NRESs to RESs (ITM Power, 2019; UKH2Mobility, 2020). Whether or not the UK meets and achieves its aims for the transport sector remains to be seen. The alternative modelling approach reduces the computing power and number of equations in current modelling. However, there are numerous constraints and variables used in alternative modelling (Seo et al., 2020; Tlili et al., 2020), and this research also aims to reduce these, making the models simpler to compute, manipulate and understand.

The principal concern of this thesis is to consider the impact of current proposals of introducing hydrogen as a transportation fuel, and so is primarily based on technical assessments. The focal point here is the most viable options for the UK's road transport network. So, the emphasis is on evaluating the system in a holistic viewpoint, rather than focusing on the in-depth detail of any component of the Hydrogen Supply Chain (HSC). This holistic approach will also help reduce the number of constraints and factors considered to determine key factors such as hydrogen demand to facilitate more realistic scenarios. A review of the approaches used to model the HSC introducing hydrogen into the UK's roads offers insights into the infrastructure issues. Limitations in the HSC literature helped to develop the dynamic model encompassing predator-prey and growth concepts instead of a static one using linear techniques.

1.4 Aim(s) and objectives

1.4.1 Research Aim

This research aims to develop a dynamic model to explore the most effective strategies for the UK's private vehicle fleet to transition to a hydrogen-based one using LV and growth concepts.

1.4.2 Research Objectives

The objectives of this research are as follows:

1) To review existing knowledge considering hydrogen infrastructure proposals for road transportation; to assess the impact of factors contributing to hydrogen demand in modelling and their input into the refuelling infrastructure requirements.
2) To propose a dynamic model assessing the introduction of HBVs into the UK's vehicle market using different scenarios.
3) To critically evaluate the model developed against current supply chain proposals and frameworks.
4) To optimise the strategies with respects to fuel economy and emissions to propose strategies for the adoption of hydrogen in the UK transportation sector.

The objectives mentioned above are investigated in this thesis. A current assessment of available technology is necessary alongside the proposals used to model the HSC and its introduction to the market to develop practical solutions for introducing hydrogen as a transportation fuel in the UK.

1.5 Originality of Research

The contributions made in this thesis can be broadly grouped together based on the modelling, overcoming limited data, and informing policies. The first contributions stemming from the thesis were the result of the modelling. LVM is a well-established model used in population dynamic modelling and in this case, it is adopted for the UK's private vehicle fleet. Since, the LVM is based on predator-prey concepts, i.e., the oscillating behaviour between competing species/technology, the classical model output was limited in this case to represent the growth and decay of conventional vehicles. The growth of conventional fuels is modelled over the past 50 years, which is then extended to incorporate the decay of conventional vehicles. Due to the environmental concerns and depletion of fossil fuels, the re-emergence of fossils fuels can be ruled out as a private vehicle fuel contender, thus the decay of conventional vehicles was also modelled for the following 50 years. Furthermore, adopting the LVM to encompass the interaction between current private vehicle fleet and AFVs. This is an aspect that is ignored in current research where the introduction of AFVs is modelled as an independent body from conventional vehicles i.e. AFVs have no impact on conventional and vice versa. Furthermore, the impact of HBVs on conventional vehicles also determined the type of strategy used.

Chapter 6 makes the final contributions in terms of modelling by extending the modified LVM into a third-order model capturing the competition between multiple fuel types. Other studies focus primarily on the introduction of hydrogen or other AFVs as single competing fuel type, however the main contribution from this chapter considers the penetration of both HBVs, NFC-EVs, and the impact on conventional vehicles. Furthermore, other studies have ignored the impact of introducing AFVs into the private vehicle market, and subsequently the impact on conventional vehicles. This enabled the analysis of the impact of both predators on conventional prey in addition to the impact of the two predators on each other. In this chapter, the HRS operating efficiency was also varied (i.e. whether the HRSs are operating at maximum capacity, 50% or well under-utilised), analysing the impact on the number of HFCVs alongside using different penetration strategies with three competing vehicle types. Some recent studies have considered the variation of HRS efficiency (Mayer et al., 2019; Tlili et al., 2020) and this thesis contributed by allowing this by altering the parameter h. By opting to use a dynamic model rather than static one, the evolution of conventional vehicles, and the impact of AFVs was considered over time. Further advantages compared to other models in literature include the model's strength, which demonstrates time reduction in simulating different scenarios and the significant reduction in computing power to achieve similar forecasts as other models.

The second broad area of contribution from the thesis was the lack of historical data and insights to forecast recent technology. AFVs are considered recent and have limited data available from the UK's official statistics, and the data for HBVs is even limited. The first-order growth model developed in chapter 3 directly over comes this issue by modelling the growth of HFCVs over 50 years using the growth rate of conventional vehicles over the last 50 years. Furthermore, the developed model was compared to other in the literature that have also forecasted the growth of HFCVs for the UK. The data used by other research is used to simulate forecasts from the modified LVM to assessing the conclusions.

The last area of contributions lies in the direction and suggested insights of the modelling informing policymakers regarding the direction of the UK's passenger vehicle fleet planning from the case study. The case study highlighted that more than 50% market share could only be achieved by overcoming significant challenges and total focus on this sector. Since AFVs will also play a role, it was suggested that 50% market share should be used as the upper limit for further research and development. The optimum strategy for the UK is a market share of 80:20 in favour of NFC-EVs to HBVs. An aggressive strategy deployed for NFC-EVs inhibits the growth of HBVs due to advantages in terms of infrastructure, current policies, and investments.

1.6 Structure of the thesis

The second chapter will cover the first objective of this thesis as outlined in section 1.4.2. The literature review initially discusses the role of modelling and optimisation in introducing hydrogen as a transportation fuel. The chapter also considers the UK as the backdrop to the case study, followed by proposals selected from the literature. Challenges associated with the design of the models are discussed, leading to the approach selected by the author to achieve the aims as outlined further in this chapter. The author proposes a single state growth model in the third chapter to assess the potential space available for alternative vehicles. The model's description is given to explain the first-order model alongside considering it from a theoretical perspective. This is followed by the implementation of the growth model for the UK's passenger vehicle fleet is described and demonstrated based on this analysis. Finally, the analysis of the results and limitations of the first-order model are presented. The fourth chapter firstly presents the second-order LVM, its description, assumptions, and governing equations. This is followed by the results section encompassing the following: modelling and testing the plausibility of the second-order model, comparison of different HRS, the number of vehicles supported by different types of stations, investment on smaller or larger stations and the case of whether investing in HFCVs will be more advantageous than HFC-REs. The conclusions and the chapter summary finally follow this. The fifth chapter covers the UK in a case study where the modified LVM is critically evaluated against current SC proposals and frameworks in accordance with objective 4. Since different studies consider different time scale/periods for the introduction of hydrogen, the following section determines a standard timeframe in which hydrogen is expected to become a dominant transportation fuel. This section followed by the formulation of penetration scenarios for hydrogen and then the results. Discussion is then followed by the chapter summary and lessons learned. The sixth chapter firstly provides an overview of the third-order model and its variants, followed by the methodology consisting of assumptions, governing equations, HRS efficiencies, model simulations, linearization of the model and optimisation. The results section is given next, followed by analysis and conclusions. The seventh chapter provides the conclusions of the thesis by summarising the contributions and highlighting areas to direct further research related to this project. Figure 1.1 provides an overview of the thesis encompassing the output of each chapter to the next.

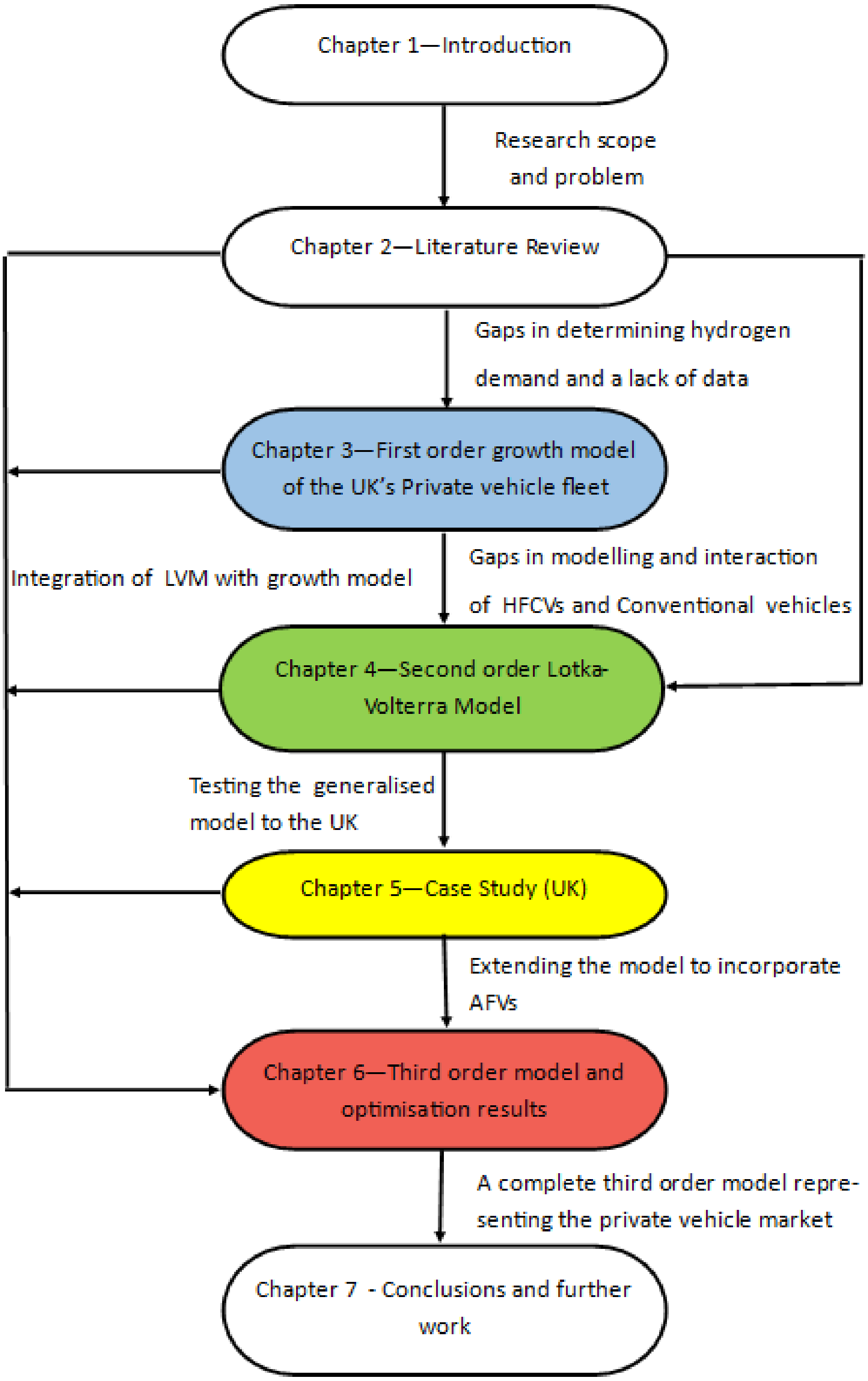


Figure 1. 1: Overall thesis structure

Chapter 2: Review of Existing Knowledge

2.1 Introduction

This chapter reviews current literature regarding the introduction of hydrogen as a competitive fuel for the private vehicle fleets in the UK. The chapter aims to identify gaps in the literature, which require further study and investigation. The concept of hydrogen in the private vehicle fleet is associated with numerous technology options that the sector must consider diversifying its fuel resources and reducing its carbon intensity. The study of introducing hydrogen for transportation has been studied from different perspectives, e.g., analysis of operating prototypes or fleets or considering the environmental and economic factors driving the adaptation of hydrogen as a transportation fuel. In this thesis, the focus is given to studies that have used a computational modelling approach. This literature review will analyse current work in generating hydrogen demand in infrastructure investment and projections made through modelling and optimisation.

The overview of the chapter is as follows: section 2.2 considers the existing approaches used to model the hydrogen supply chain and the main conclusions drawn. It covers optimisation-, geographic information-, energy system- and system dynamics-based approaches. Section 2.3 covers modelling approaches and decisions made to determine the hydrogen demand, including calculating the hydrogen demand per year, penetration strategy for HFCVs and scenarios, HRS operating efficiency, and HRS timeframe. Section 2.4 considers the initial and long-term hydrogen demand based on current policies and projections, while section 2.5 outlines the implications on the modelling representation of hydrogen demand. Section 2.6 provides an overview of the UK's case study and why it is appropriate for this study. And, finally, section 2.7 considers the implications and research gaps in the literature.

2.2 Forecasting hydrogen's role as a fuel

Representing the integration of hydrogen into the transport system has significantly evolved over the last two decades, which is self-evident from the numerous reviews in this area (Dagdougui, 2012; Li et al., 2019). Dagdougui (2012) classified the models and approaches into three distinct categories: optimisation methods, GIS-based approaches, and assessment plans toward the transition to hydrogen infrastructure. The third category contained other types of models and those that utilised both optimisation and GIS-based models. However, in a different paper, Agnolucci and McDowall (2013) critically analysed the literature through spatial scales encompassing optimisation models. They split the optimisation modelling section into three (1) the type of modelling family, (2) the area of consideration, e.g. regional or national, (3) spatial representation of refuelling stations (Agnolucci and McDowall, 2013). Besides, the advantage of this approach allowed the inclusion of a wide breadth of models. In a review paper by the author, a section for system dynamics studies was also included alongside where the inclusion of policymaking is considered on system control with regards to selected metrics (Maryam, 2017). Li et al. (2019) conducted a comprehensive review of the optimisation models for HSC network design, identifying the scope of entities and technologies studied previously. In a different review paper, the global hydrogen supply chain was considered from production to storage, and delivery to utilisation. Whilst hydrogen has huge potential to be utilised as a carbon-free fuel, however current infrastructure and technologies are under-developed (Ratnakar et al., 2021).

From the previous review conducted, different mathematical approaches and frameworks have modelled the introduction of hydrogen for road transportation with various factors in mind, in particular, cost (Baufumé et al., 2013a; Robles et al., 2020; Seo et al., 2020). In some cases, the optimal solution is sought based on the minimisation or maximisation of a relevant metric such as cost, or emissions considering the entire economy. It is important to attain equilibrium in decisions with regards to hydrogen production, storage, and distribution. These form various components of the supply chain. Besides, the type of strategy employed will determine the feedstock, production and transportation options utilised, e.g. centralised (Seo et al., 2020), decentralised (Almansoori and Shah, 2012), or on-site (Gim and Yoon, 2012) production. So, one of the key criteria for implementing an infrastructure to establish a new transportation fuel is the demand for the fuel (Robles et al., 2020). Vehicle manufacturers are reluctant to build fleets and opt for prototype and small fleets to run trials and gather data for transition. It is difficult to justify investment in a hydrogen refuelling station (HRS) network with little or no vehicles alongside a customer base (Liu et al., 2016). Integrating hydrogen into the transport sector at whatever level of penetration will require substantial investment by various stakeholders, from vehicle manufacturers to the government (UKH2Mobility, 2013, 2020). While the research conducted for this thesis project is not a hydrogen supply chain (HSC) focused, it will consider HSC modelling approaches used in the literature in addition to forecasting and dynamic modelling to understand the challenges associated with utilising hydrogen. The following few sections will summarise the review paper on hydrogen supply chain and infrastructure modelling written by the author (Maryam, 2017).

2.2.1 Optimisation based approaches

Hydrogen can be produced from a number of feedstock utilising different techniques such as electrolyses, steam methane reformation (SMR) etc. (Abbasi and Abbasi, 2011; Ajayi-Oyakhire, 2012; Wickham et al., 2022). As a result of this, researchers have pre-selected HSC for the purpose of modelling the hydrogen demand and forecast for near- and long-term future. Table 2.1 gives an overview of the different types of optimisation-based approaches used by researchers. A number of design variables and operations of the HSC can be selected and analysed using optimisation models i.e. steady state or dynamic; deterministic or stochastic (Almansoori and Shah, 2006, 2009; Murthy Konda et al., 2011; Dayhim et al., 2014; Islam et al., 2016). The advantage of using optimisation techniques is that they deal with the "how to" aspect of the problem rather than the "What if" aspect (Hiremath et al., 2007; Bolat and Thiel, 2014).

Unlike optimisation approaches where the optimum pathway is selected, Mixed Integer Linear Programming (MILP) deal with approaches where some of the variables are restricted to be integer allowing a number of different design variables to be taken into account (Ochoa Bique and Zondervan, 2018; Larrosa et al., 2020). The advantage of utilising MILP-based approaches is that they offer a flexible tool to researchers investigating a number of different objectives such as identifying appropriate locations (Wang and Lin, 2009); most economical pathway (Ingason et al., 2008); evaluation of the economic potential alongside the infrastructure requirements of a pathway for a certain location (Parker et al., 2010); to identify the least-cost pathway (Lin et al., 2008; Almansoori and Betancourt-Torcat, 2016a; Woo et al., 2016; Ochoa Bique and Zondervan, 2018); and the selection of optimal designs of a low-carbon HSC (Gabrielli et al., 2020).

Multi-period optimisation models solve known parameters and different echelons simultaneously. This allows decisions and trade-offs to be made simultaneously between different periods. In recent literature, a multi-period HSC was developed to analyse the impact of current infrastructure on aspects of the development of hydrogen technology. The HSC encompassed the assessment of NG and by-product hydrogen to assess the most efficient use of different hydrogen technologies over time. To overcome the uncertainties of the estimation of hydrogen demand, the study incorporated the governmental targeted value of hydrogen supply, and performed a sensitivity analysis on the total hydrogen demand (Yoon et al., 2022). In a different study, stochastic demand was employed to estimate the probability distributions of potential outcomes by varying inputs over time detecting critical factors contributing to the design of an optimal network (Dayhim et al., 2014). Another approach used scenarios to calculate uncertainty resulting from long-term variation in hydrogen demand (Almansoori and Shah, 2012). The production of hydrogen and development of the corresponding storage facilities and transportation modes are directly linked to the proportional hydrogen demand as determined by demand-driven models (Almansoori and Shah, 2012; Dayhim et al., 2014; Yoon et al., 2022).

Multi-objective optimisation problems look to optimise more than one objective function simultaneously. This approach is ideal where optimal decisions are required by making trade-offs between two or more conflicting objectives (Bae et al., 2021). A number of studies in the HSC area have utilised this approach, where authors have investigated the best solutions considering a number of variables such as cost, global warming and safety risk (Li et al., 2008; Guillén-Gosálbez et al., 2010; Murthy Konda et al., 2011; Akgul et al., 2012; Sabio et al., 2012; De-León Almaraz et al., 2013; Kumar et al., 2016). In contrast to MILP models mentioned previously, cost efficiency and safety were considered using a multi-objective optimisation approach. Demand uncertainty was assessed by analysing the deterministic and stochastic solutions (Kim and Moon, 2008; Martín, 2016; MathWorks, 2016).

A single objective with many constraints may not adequately represent the problem. Having more objectives will complicate the trade-offs and are less easily quantified (MathWorks, 2016). Multi-objective optimisation problems do not usually have a single optimum solution for the all the objectives simultaneously as the objectives are usually in conflict with each other (Bae et al., 2021), e.g. reducing cost and the environmental impact. This results in a group of efficient solutions that fit the problem and a number of technique have been used by researchers to calculate the group of efficient points: aggregation of objectives, e-constraints, compromise programming, etc. (Brey et al., 2006, 2007; Mavrotas, 2009; De-León Almaraz et al., 2015a).

The development of HSC pathways is a necessary measure to analyse the behaviour of the energy system across the whole energy system. To achieve this, the models proposed need to give a precise account of the pathways linked with the techno-economic assumptions made. Furthermore, the models proposed in this section are static and SCs are often complicated and time-dependant, so therefore it is more likely that to accurately represent the HSC then a dynamic model must be proposed. Other types of optimisation models such as System Dynamics (SD) are perhaps better at representing the interactions of a SC than linear modelling.

Table 2. 1: An overview of the different types of optimisation approaches

Mathematical optimisation approach	Characteristics	References
Mixed Integer Linear Programming (MILP)	All parameters are integers and fast to resolve. Reduced computing time and is a rigorous, flexible approach with extensive modelling capacity.	(De-León Almaraz et al., 2013; Almansoori and Betancourt-Torcat, 2016b; Ochoa Bique and Zondervan, 2018; d'Amore et al., 2019; Gabrielli et al., 2020; Yang et al., 2020)
Mixed integer non-linear programming (MINLP)	Non-integer parameters are used and can be directly implemented in a modelling language. Increase in simulation time and are often complicated.	(De-León Almaraz et al., 2015b)
Multi-period problems (MPP)	All parameters are known and different echelons are solved simultaneously. Decisions and trade-offs can be made simultaneously between different periods. Can complicate the model.	(Almansoori and Shah, 2009; Dayhim et al., 2014; Bae et al., 2020; Yoon et al., 2022)
Multi-objective problem (MOP)	Uncertain quantities characterised by probability distributions. Different objective parameters can be analysed and traded off. Can overly complicate the model.	(Mavrotas, 2009; Guillén-Gosálbez et al., 2010; Kumar et al., 2016; Robles et al., 2020; Bae et al., 2021)

2.2.2 Geographic Information System (GIS) based approaches

One alternative approach to optimisation-based approaches is the Geographical Information System (GIS) based approaches (Table 2.2). Models incorporating GIS are dependent on national or regional-specific conditions such as the population, size, or location etc. whereas optimisation approaches are more generic. Researchers have begun to use GIS packages more frequently and often include it as an element within a modelling system for SC management (SCM) (De-León Almaraz et al, 2015b).

A number of researchers have used an energy system optimisation framework to analyse long-term hydrogen fuel and vehicle adoption e.g. MARKAL/TIMES (Strachan et al., 2009; Yang and Ogden, 2013; Balta-Ozkan and Baldwin, 2013; Gerboni and Grosso, 2016). These frameworks enable the optimisation of the entire energy system so that competition for primary energy resources for the consideration of different energy services. Like optimisation approaches, there are many variants available with an important role to play within the energy system, further developments are required to enhance the analytical tools available to assess different aspects (Pfenninger et al., 2014; Hall and Buckley, 2016). Utilising GIS, researchers have been able to identify potential hydrogen demand centres as well as supply locations and the infrastructure to link them. Some studies have combined GIS with other approaches such as mathematical optimisation methods (Marcoulaki et al., 2012), ArcGIS (De-León Almaraz et al., 2015a), heuristics algorithm (Kuby et al., 2009), multi-criteria decision making (Messaoudi et al., 2019), and agent based model with swarm optimisation (Thiel, 2020). While these offer a more enhanced method to explore various aspects of the HSC, the computing power and storage capacity adds to the complexity of the model leading assumptions or limited scenarios (Messaoudi et al., 2019).

Some of the limitations of GIS based approaches is the complexity of the systems making them expensive, it is also difficult to integrate the system with traditional maps to gain meaningful information. Like the system, the data and information collected can be quite difficult to analyse due to the complexity and the presentation of the data in GIS system may also not be organised for easy end-user consumption (Rehman, 2018).

Table 2. 2: An overview of GIS-based approaches adapted from (Maryam, 2017).

Type of model	Characteristics	References
GIS-based model	GIS – Geographical Information system environment. These rely on national or regional-specific information such as population, size, availability of resources etc., and can help identify specific conditions for different geographic scales.	(Reuß et al., 2019; Baufumé et al., 2013b; Johnson et al., 2008)
GIS based MCDM	Multi-Criteria Decision Making with GIS	(Messaoudi et al., 2019)
Cluster Strategy	Cluster strategy – coordinated introduction of hydrogen vehicles and refuelling infrastructure in a few geographic areas.	(Ogden and Nicholas, 2011)
MOREHyS (model for optimisation of regional hydrogen supply) model	MOREHyS – a tool to access to introduction of hydrogen as vehicle fuel by means of energy system analysis.	(Ball et al., 2007)
STREET (Spatially and Temporally Resolved Energy and Environment Tool)	STREET – system planning tool operating at the highest level of spatial detail and integrates multiple considerations.	(Stephens-Romero et al., 2010)
GIS + Heuristics algorithm	Operations research (OR) models.	(Kuby et al., 2009)
GIS + ABM + Swarm Optimisation	Agent based model integrating particle swarm optimisation and GIS	(Thiel, 2020)
GIS – MARKAL (MARKet Allocation)	MARKAL – a linear optimisation model. Its strengths are in analysing resource competition in	(Balta-Ozkan and Baldwin, 2013; Strachan et al., 2009; Tseng et al., 2005)

	economics, engineering, environment, and energy terms.	
H2TIMES	H2TIMES – a quasi-spatial model	(Yang and Ogden, 2013)
MOP - ArcGIS	ArcGIS – A GIS used to organise, analyse, and map spatial data.	(De-León Almaraz et al., 2015b)
Stochastic optimisation + GIS	Stochastic – a systematic search for optimal and near-optimal solutions.	(Marcoulaki et al., 2012)

Johnson et al. (2008) further highlights this by suggesting that whilst GIS based approaches offer valuable insights into regional infrastructural development, the spatial complexity inherent in individual locations is often overlooked. So, therefore utilising GIS on its own is limited, however by integrating it with other models increases the complexity and amount of computing power and storage capacity for data.

2.2.3 System Dynamic (SD) based approaches

Complex systems, i.e., SCs can be modelled by System Dynamics (SD), which is a mathematical modelling technique (table 2.3). SD combines a number of techniques from non-linear dynamics to feedback control theory using computer simulations as the measure (Sterman, John D, 2000). This tool is useful in studying the influences of policy making on system control while encompassing constraints from the methodology on structural characteristics. Changes in the system behaviour are considered over time especially dynamic behaviour with the feedback structure identifying the cause of dynamic change (Borshchev and Filippov, 2004; Park et al., 2011a). SD overcomes the limitations of conventional statistical methods, which focus on correlations primarily. For this reason, SD is often employed across disciplines in particular, the case of introducing recent technologies and innovations. Furthermore, it is also useful in assessing the inter-related relationship between multiple variables through simulations (Sterman, John D, 2000).

The product diffusion model (PDM) focuses on the development of a new product throughout the expected life cycle from entry to the market taking customers' choices and behaviours into account to better inform the production marketing and finance phases (Wang and Wang, 2016a). The Bass Diffusion Model (BDM) is a well-established diffusion model, which describes the s-shape trajectory of a new product with significant parameters, e.g. the innovation, and imitation factors (Meade and Islam, 2006). However, this model does not take external variables, i.e. marketing into account, nor the influence of external variables on the innovation and imitation factors over time. As a result of this, a generalised bass diffusion model (GBDM) is often used, where another variable is added taking the impact of decision variables on the adoption of the conditional probability with respect to time (Park et al., 2011a). One of the disadvantages of applying the BDM in a real-world problem is the lack of data to estimate the model's parameters. This is due to the forecasting of a new product that is yet to reach the market. The GBDM coupled with historical time series data is yet to be utilised in the study of HFCV forecast.

Since the early work of Bass in 1969, the PDM has been modified by researchers to reflect real-life complexity of the market (Wang and Wang, 2016b). The research conducted in this thesis proposes a framework/model of the deployment and competition of HBVs into the UK's passenger vehicle sector. Therefore, the PDM is unable to suitably clarify the diffusion behaviour and mechanism in a mutually competitive market. The representation of mutual interaction is necessary and for this reason the LVM is considered. The LVM is based on the growth development curve and is used to explore the interactions between two or more diverse competitors (Wang and Wang, 2016b).

Table 2. 3: An overview of System Dynamics (SD) models.

Type of Model	Characteristics	Reference
System dynamics (SD)	This is the study of dynamic behaviour of a system in relation to time.	(Melaina, 2003)
Long range Energy Alternatives Planning technology database (LEAP).	This is a dynamic linear programming tool with an annual time step.	(Amoo and Fagbenle, 2014)
The Bass Diffusion Model (BDM)	The model describes the s-shape penetration curve of how new product penetrate markets as an interaction between consumers and potential consumers.	(Meyer and Winebrake, 2009)
Generalised Bass Diffusion Model (GBDM)	The BDM is extended to include external variables.	(Park et al., 2011a)
Dynamic GTAP model	This is a global computable equilibrium model (CGE) and is typically utilised to examine related to free trade.	(Lee, 2014a)
Agent-based modelling (ABM)	ABM is a tool that studies social systems from the complex adaptive system perspective.	(Janssen, 2005; Keles et al., 2008)
Product Diffusion Model (PDM)	Forecasts the market penetration of new products by considering the lifecycle.	(Wang and Wang, 2016a; Singhal et al., 2020)

The Lotka-Volterra (LV) equations have been used in a number of research areas to model competing technologies, although originally defined to analysis problems concerning population dynamics (Gokmen et al., 2015). These set of differential equations have been studied extensively in relation to various systems (He et al., 2012; Miranda and Lima, 2013; Marasco et al., 2016; Hung et al., 2014, 2017; Mao et al., 2020; Mohammed et al., 2021).

Further developments have led the use of these equations as a theoretical framework to nonlinear systems, computational tools leading to generalisation of the LV equations in literature in order to bring their representation closer to reality (Filho et al., 2005; Liu and Guo, 2021). The primary purpose of the LV equations is to deal with the growth and interactions between species, and for the simplest case of a predator-prey is complex. One of the disadvantages of the LVM is the oversimplification, where it lacks robustness and often demonstrates mathematical instability against various model modifications and variations (He et al., 2012). However, the LVM is often modified and applied to other fields, i.e. LVM was successfully used to explore the behaviour of the competition between different size silicon wafers in the IC Foundry industry (Chiang, 2012). In another case, the LVM was used to analyse the competition between smart TVs and flat panel TVs, where flat TVs cover the usual function of a TV and a smart TV's use can be increased through apps and other functions. In addition to the dynamic competition between Android (customisable system that can be modified to user's preference – partly open source unlike iOS) and iOS smartphone operating systems (OS) (Wang and Wang, 2016b). Maurer and Huberman in 2003 used predator-prey concepts to develop a dynamical model of web site growth to analyse the competition among web sites and their impact on the nature of markets (Maurer and Huberman, 2003). In 2012, conducted a study investigating competition between different types of TVs based on a tripartite dynamic competition using LV concepts (Kreng et al., 2012). Marasco et al. (2016) assessed competition in the marketplace using LV concepts to describe and forecast market. Mao et al. (2020) applied the Grey-LVM to quantitatively analyse and predict the impact of commercial banks' online payment system on the development of third-party online payment systems in terms of cooperation and competition relationships. In a more recent study, the researchers made an analytical appraisal of the dynamic behaviour of LV based models of COVID-19 (Mohammed et al., 2021). Dynamic models incorporating growth theory, performance of investors, growth of population and capital stock accumulations are quite popular in assessing the behaviour of SCs (Lee, 2014b; Pasaoglu et al., 2016).

Utilising SD to model the introduction of hydrogen as a transportation fuel opens many exciting possibilities in integrating various tools and models to give alternative models to those discussed earlier. However, lack of historical data of HFCVs is a limitation in using forecasting models. Yet, developing economic growth model incorporating data from conventional vehicles may overcome this issue. It is also possible to use models such as the Lotka-Volterra Model (LVM) to analyse the relationship between different types of vehicles and their introduction into the market. This is important when it comes to introducing HBVs into market because of the lack of data available.

2.3 Hydrogen Demand Modelling

Estimation of the hydrogen demand is a dynamic process involving several factors that are open to interpretation. The following sections examine hydrogen demand more closely determining the assumptions underpinning those projections. Hydrogen demand, in a sense is just like any other fuel demand. The quantity of hydrogen is based on the need to fuel HFCVs. So, in other words, it is positively reinforced in a feedback loop by the number of HFCVs, and vice versa. One of the major limitations of estimating the hydrogen demand is the agreement of saturation point for HFCVs. Table 2.1 summarises the main variables that researchers have considered when developing their respected models. The following few sections are as follows (1) Calculating the hydrogen demand per year, (2) Penetration strategy for HFCVs and magnitude of demand, (3) HRS operating efficiency, and (4) HRS timeframe.

Table 2. 1: Different decisions involved in determining the hydrogen demand

Model Type	Year Period	Scenarios	Penetration strategy	HRS Operating efficiency	Ref
Multi-period optimisation	2020 - 2050	Y	Y	-	(Yoon et al., 2022)
Spatially solved optimisation	2020 - 2050	Y	Y	-	(Wickham et al., 2022)
Bi-objective optimal design (MILP + GAMS)	2035 - 2050	Y	-	-	(Carrera and Azzaro-Pantel, 2021)
MILP Optimisation	-	Y	Y	-	(Seo et al., 2020)
Geospatial model	- 2035	Y	Y	Y	(Tlili et al., 2020)
Optimisation	2020 - 2050	Y	-	Y	(Talebian et al., 2019a)

Energy and economic comparison	2015 - 2050	Y	Y	Y	(Mayer et al., 2019)
MILP + AIMMS	2030/2050	Y	Y	-	(Ochoa Bique and Zondervan, 2018)
Logistic Diffusion Model	2020-2070	Y	Y	-	(Moreno-Benito et al., 2017)
A short-term analysis	2016-2055	Y	Y	-	(Liu et al., 2016)
MILP Optimisation	2040	Y	-	-	(Woo et al., 2016)
Mixed methods approach	2015-2030	-	-	-	(Southall and Khare, 2016)
UK MARKAL	2050	Y	-	-	(Balta-Ozkan and Baldwin, 2013)
UKH2Mobility Report	2015-2030	-	-	-	(UKH2Mobility, 2013)
Multi-period stochastic model	2005 - 2030	Y	Y	-	(Almansoori and Shah, 2012)
Optimisation	-	Y	Y	-	(Dagdougui et al., 2012)
Bi-criterion MILP		-	-	-	(Guillén-Gosálbez et al., 2010)
GIS MARKAL	-	Y	-	-	(Strachan et al., 2009)
GIS based technoeconomic model	-	Y	Y	-	(Johnson et al., 2008)

2.3.1 Calculating the hydrogen demand per year

Researchers have often considered the cost of implementing a new hydrogen infrastructure and the environmental implications as primary objectives of proposed models (Yang and Ogden, 2013; Dayhim et al., 2014). Both factors hinge on the estimation of hydrogen demand in majority of models proposed by both researchers and government roadmaps (UKH2Mobility, 2013; European Commission, 2020). The estimation of hydrogen demand directly influences other key decisions of any SC or the type of infrastructure established. As a result, this section considers the approaches used in the literature to quantify the hydrogen demand.

Some studies consider the value of hydrogen demand exogenously as a model input. For instance, De-León Almaraz et al., (2013, 2015) developed a deterministic demand for transportation system. Here the hydrogen demand was estimated from the product of fuel economy, the average distance travelled, and the total number of vehicles. Similarly, Ochoa Bique and Zondervan, (2018) calculated the hydrogen demand for the year 2050 by considering the average distance travelled and the transport fuel economy assuming HFCVs will gain 30% of the market. The HFCV penetration rate was also multiplied by the average number of privately owned vehicles per 1000 people. Carrera and Azzaro-Pantel, (2021) also considered a deterministic demand for both methane and hydrogen in their bi-objective optimal design of hydrogen and methane SCs. For methane, the total demand was met by the production of methane from each grid, whereas, for the hydrogen demand, the quantity of hydrogen required to satisfy the methane production as feedstock was included with the demand for hydrogen as an end-product. The deterministic approach has been the most common method to estimate the hydrogen demand in the literature for the past decade (see. Fig.2.1). Alternatively, the hydrogen demand can be endogenized by modelling the behaviour of the sector's stakeholders during the transition phase (Keles et al., 2008). However, the cost of hydrogen, initial vehicle costs, station availability and subsidies will strongly influence the model's preferences and benefits.

Alternatively, hydrogen demand has also been calculated by considering the required fuel for a HFCV and multiplying this by the number of expected HFCVs in a year. This was the case for Ontario where the estimation of hydrogen demand for a HFCV was based on the specification data of GM Equinox HFCV model, while the number of HFCVs is calculated from the projections of HFCVs estimated through three scenarios (Liu et al., 2012). The advantage of using this method is that it reduces the complexity of the modelling e.g. vehicle efficiency, and distance travelled are no longer necessary as the above-mentioned studies. Furthermore, a different approach is to consider the traffic volume of a region to determine the average travelling distance. For instance, Woo et al. (2016) estimated the hydrogen demand for a biomass hydrogen supply chain by considering the expected number of HFCVs, their conversion efficiencies and the traffic volume expected at Jeju Island. The hydrogen demand for 2040 was generated by multiplying the resident population of each region by monthly traffic rate.

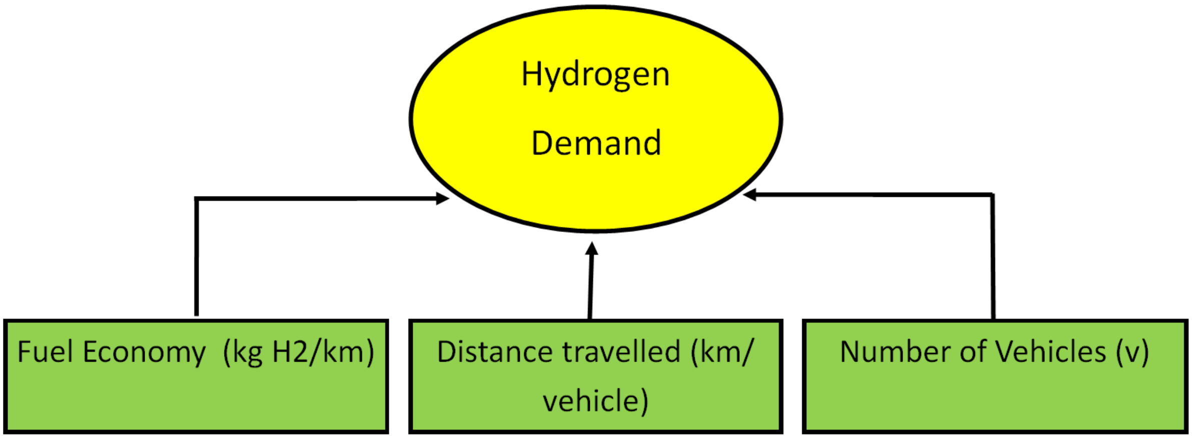


Figure 2. 1: Exogeneous hydrogen demand (Almansoori and Shah, 2006; De-León Almaraz et al., 2013, 2015b; Talebian et al., 2019b)

Agnolucci and McDowall (2013) observed that similarly to other new technologies, the adoption of hydrogen is expected to follow the same s-shaped trajectory (see. Fig.2.2). The s-curve is defined by three parameters, namely, the saturation point, the anchoring point i.e. start of transition or midway, when half the market share has been reached, and the duration of transition. Other studies have also considered the s- shaped trajectory (Almansoori and Shah, 2009; Park et al., 2011a; Yoon et al., 2022). Here, it suggests that the number of HFCVs are adopted rapidly after initial barriers are overcome to the saturation point.

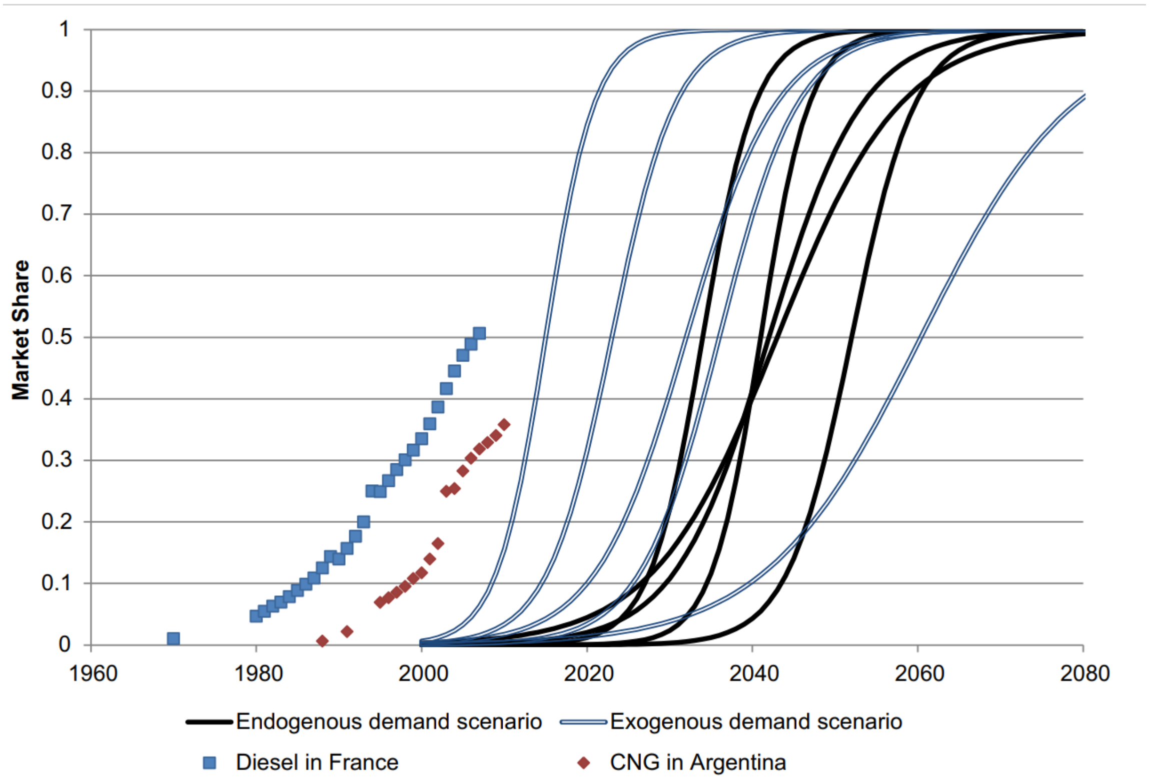


Figure 2. 2: Comparison of endogenous and exogenous hydrogen demand fitted into a s-shaped curve with historical data of France and Argentina (Agnolucci and McDowall, 2013)

Some researchers have also considered the geographical profile or spatial allocation (Agnolucci and McDowall, 2013) in estimating the hydrogen demand. Yang et al. (2020) estimated the hydrogen demand by developing a forecast model that considers the actual collected data based on the existing hydrogen demand forecasting methods. The distribution of the population is considered as the number of HFCVs in relation to the geographical region (urban v rural) and population density. Like many papers, scenarios approach was utilised to encompass the uncertainty aspect of hydrogen demand. In a different paper, the hydrogen demand was estimated through customer's profile and demand geographical distribution. The model assumes that each geographic region has its own deterministic demand, where the demand must be met by local production and/or imports from neighbouring grids (Almansoori and Betancourt-Torcat, 2016a). Similarly, the hydrogen demand was calculated by dividing the landscape of Germany into 16 grid points. The hydrogen demand for each grid point must be satisfied by local production, and if not, then imported from neighbouring grids (Ochoa Bique and Zondervan, 2018). In a different case, the hydrogen demand was also calculated for each region was by the product of the number of HFCVs in a particular region and time, the fuel economy of the HFCV, and the annual average mileage, all divided by the number of days in a year (Yoon et al., 2022). In another instance, the hydrogen demand was fixed as an input parameter reaching a maximum capacity of 100 tonnes per day per regional use (Lahnaoui et al., 2019). The issue with splitting the hydrogen demand is that it is assumed that the constraints on each region are the same, and that the adoption of hydrogen has evolved concurrently across all regions. This is a problematic assumption as it ignores geographic, and economic differences, alongside investments already implemented in some areas.

In a different approach, Dagdougui et al. (2012) estimated the hydrogen demand considered the number of HRSs based on current supply of fuel to conventional petrol stations. Murthy Konda et al. (2011) estimated the hydrogen demand (kg/day) considering the total number of light-duty vehicles multiplied by the percentage of LDVs in the regional market, multiplied by the total distance travelled (km/day) and the fuel economy (kg/km). In this case, the temporal aspect of the hydrogen demand was encompassed by increasing the market share with time. Kim et al. (2008) estimated the hydrogen demand by calculating HFCV share in the future transportation energy demand after determining the future energy & economy growth rate. This was then used to estimate the hydrogen demand, which was used to estimate the regional hydrogen demand density based on vehicle population demand and census data on vehicle types and region. Wickham et al., (2022) used a similar approach to Kim et al. (2008) to determine the hydrogen demand for each grid point. However, in this case the hydrogen demand was calculated by considering the annual fuel demand for road transport leading up to 2018. This represented the total hydrogen demand for transport in each time period assuming 100% market penetration. Dayhim et al. (2014) proposed a spatially demand model to estimate the hydrogen demand. The proposed model took households into account as consumers instead of individuals due to the possibility of every household having more than one vehicle.

Estimation of the hydrogen demand is a critical factor when it comes to modelling the HRS infrastructure/SCs of the future. Have a stringent demand will lead to an underestimation planning, and investment, while an overly zealous demand will result in under-utilisation of refuelling stations and other components with little demand. To extrapolate sensible demands for hydrogen then several areas need to align, such as the scenarios selected, the penetration rate of hydrogen as a fuel for passenger vehicles, market share etc.

2.3.2 Penetration strategy for HFCVs and scenarios

This section considers the penetration strategies employed by researchers, the number, and the type of scenarios selected projecting different forecasts of hydrogen penetration in the passenger vehicle sector. Different penetration strategies are often depicted as market share of HFCVs in relation to the vehicle market, e.g. the implementation of HFCVs in France were considered using 4 scenarios with a deterministic demand. The scenarios proposed assumed that 1% of the vehicle fleet in France at 2012 levels would be covered by HFCVs in 2020, 7.5% in 2030, 17.5% in 2040, and 25% in 2050. In this case, the hydrogen penetration rate was used synonymously with hydrogen market share with a low market share indicating low penetration rate and a larger market share indicating a high penetration rate (De-León Almaraz et al., 2015b). The number of scenarios varies study to study: 6 scenarios (Liu et al., 2012), 5 scenarios (Johnson et al., 2008), 4 scenarios (Woo et al., 2016; Seo et al., 2020; Yoon et al., 2022), and 3 scenarios (Murthy Konda et al., 2011; Dagdougui et al., 2012; Iordache et al., 2017; Tlili et al., 2020). Alternatively, Kim et al. (2008) considered hydrogen demand as 20% above average, average and 20% below average growth of the average values of three scenarios, as opposed to penetration scenarios that vary in accordance to the market share.

Scenarios have been used to reflect an aspect of the HSC or the entire SC. Lahnaoui et al. (2019) optimised the hydrogen transport system in terms of the transport mode proposing a market share of 2.4% by 2030 with an average demand of 338/379 tonnes per day. Similarly, Woo et al. (2016) used 4 scenarios to represent different hydrogen storage and import policies e.g. inventory and import policies are used to align demand, increasing the number of gasification plants to meet demand summer etc. On the other hand, Seo et al. (2020) used a MILP optimisation model to design and optimise the hydrogen supply chain (HSC) from supplier to end use, but from the perspective centralised and decentralised systems rather than a particular supply chain. In this case four scenarios were considered for each centralised and decentralised storage systems. South Korea was used as a backdrop with hydrogen expected to attain market share of 15-30%. A key outcome was the switch in strategy from decentralised to centralised storage system when the market share reaches 20% for HFCVs. Ball et al. (2007) also found that a centralised infrastructure was economic under dispersed liquid hydrogen demand in Germany's national energy system using an optimising modelling approach. Five scenarios were proposed which were split into two sections: infrastructure scenarios, i.e. 'Urban', 'rural', and 'Urban liquid hydrogen'; and energy price scenarios i.e. urban high gas price with and without a carbon dioxide cap. In some cases, scenarios are utilised to represent the temporal aspect of the models. The scenarios selected often provide a snapshot of HFCV's forecast in one year, a number of these forecasts are provided to assess the temporal growth of HFCVs (Talebian et al., 2019a). Similarly, the temporal aspect was taken into account by considering 4 periods from 2020 to 2050 with a 10 year step for each (Robles et al., 2020) and across 6 time-periods to facilitate long-term multi-period modelling (Rahmouni et al., 2016). However, Johnson et al. (2008) did not take the temporal aspect into account opting to focus on implementing GIS to calculate the location and magnitude of hydrogen demand and optimise the placement and extent of hydrogen production and distribution facilities. In a different case, Yoon et al (2022) considered the introduction of hydrogen by utilising the existing NG pipeline infrastructure and by-product hydrogen. Four different scenarios were outlined: in the first case there is no existing infrastructure, for the second case by-product hydrogen is available, but the NG pipeline network is not developed fully, the third case represents the option where the NG pipeline network is readily available and fully developed but without by-product hydrogen, and for the final case both by-product hydrogen and a fully developed NG infrastructure are available (Yoon et al., 2022).

Some studies have introduced HFCVs by considering previous disruptive technologies assuming similar barriers for HFCVs. Agnolucci et al. (2013) used a logistic diffusion model to generate a plausible scenario of diffusion of hydrogen into the transport sector. Hydrogen vehicles were also assumed to achieve 100% of the stock. Further to this, the introduction of hydrogen was simulated at the pace of other similar technologies into the market such as AFVs. In a different study, the hydrogen was calculated in two steps, the first calculated the electricity produced from renewable energy sources (RES) in Ecuador, and the second was used to calculate the corresponding hydrogen (Posso et al., 2016). This does assume that all the renewable electricity in Ecuador will be used for the purpose of producing green hydrogen. For Romania, Iordache et al. (2017) assumed that a minimal and critical HRS network is a prerequisite for the initiation of using hydrogen for road transportation. Three scenarios were assumed, each starting with 3 HRS leading to 150, 250 and 350 stations.

This section has identified several approaches that researchers have used when establishing the number of scenarios, the penetration strategy of hydrogen and the market share. Very few researchers have considered a 100% market share for HFCVs in recent literature. The maximum demand of hydrogen for the UK's transport was selected in a recent study, albeit the penetration followed the 'S' shaped trajectory (Wickham et al., 2022). A 100% market share was attained by 2045 in a different study (Rahmouni et al., 2016), and 100% of the stock of another (Agnolucci et al., 2013). Others have used 50% market share (Seo et al., 2020), 25% (De-León Almaraz et al., 2015b) as the best-case scenario etc. So, therefore policies of the country, current investment and implementation alongside other practicalities must be considered when outlining different scenarios.

2.3.3 HRS operating efficiency

Hydrogen demand as mentioned in the earlier sections is calculated through the number of HFCVs. This can also be determined from the number of HRSs and the maximum operating capacity. HRSs are highly unlikely to operate at maximum capacity and only at certain peak times. Mayer et al. (2019) assumed that the HRS will operate at maximum capacity on Friday peak hour, so one hr/wk. The average daily capacity is defined at 100% and the station performance was also considered for 2, 4, 10, 25, 50, and 100%. An average refuelling capacity of 4.6kg is used to determine the daily hydrogen demand at a station. Tlili et al. (2020) assumed that the hydrogen demand is greater in the summer and lower in winter by 10%. Also, HFCVs are expected to be refuelled towards the end of the week rather than the start due to the weekend, whilst the demand is also area dependent and a maximum utilisation of 70% was assumed for each station under different situations. This can lead to under-utilisation and over-utilisation of some HRSs. Thus, it is a key factor in modelling the hydrogen demand as it can lead to unsuitable projections. The daily variation in the HRS efficiency is difficult to predict, however some papers have varied the operating efficiency as upper and lower limit in each scenario. Talebian et al. (2019) assumed that the operating efficiency of the HRSs is the same as the maximum capacity of each station (150, 500, 1000, and 1500 kg/day) and minimum capacity was set at the stations operating at 10% efficiency of the maximum capacity.

2.3.4 HRS Timeframe

The UK has initiated a policy to reduce the net carbon account for the year 2050 by at least 100% lower than the 1990 baseline (legislation.gov.uk, 2019a). Many studies have considered the temporal aspect of introducing hydrogen as a transportation fuel. Many studies have used a timeframe up to the year 2050 of varying hydrogen proportion of the vehicle market (Balta-Ozkan and Baldwin, 2013; Mayer et al., 2019; Talebian et al., 2019b; Yoon et al., 2022). Some studies have considered a shorter timeframe of 2035 (Tlili et al., 2020), 2030 (Almansoori and

Shah, 2012; Southall and Khare, 2016). Other studies considered a longer timeframe where 50% of the vehicles were HFCVs by 2070 (Moreno-Benito et al., 2017) and 2055 (Liu et al., 2016). Models that have taken the temporal aspect into account have notably considered the quantity of emissions that need to be reduced by a certain period (Balta-Ozkan and Baldwin, 2013). Others have provided a snapshot of either a model with determined hydrogen demand at different intervals (Almansoori and Shah, 2006; Strachan et al., 2009; Yoon et al., 2022) or of a particular HSC such as coal-based infrastructure (Johnson et al., 2008).

2.4 Hydrogen Demand forecast based on current policies and projects

Current research and policies indicate that many countries/states are investing in a pre-commercialisation infrastructure to create an artificial demand for hydrogen, thus overcoming the chicken and egg problem (CaFCP, 2018; Campíñez-Romero et al., 2018a; Leibowicz, 2018). This also gives a chance to run the vehicles comparing the performance, availability, and actual emissions/efficiencies to that of conventional vehicles. Several countries have developed a roadmap strategy involving the government and several key stakeholders, who act as a co-ordinating agency outlining specific milestones and approaches tackling key issues with regards to HBVs and the corresponding infrastructure (UKH2Mobility, 2013; SHHP, 2016; CaFCP, 2018c; Kyodo News, 2018). For example, California has set a target of 100 HRS to ensure successful commercialisation for HFCVs by early adopters (CaFCP, 2018c). The first few stations were built during 2000-2008 period, where federal and local government were able to provide funding making the transition look promising.

This strategy is quite popular and used in other countries too, e.g. the European Union ‘HyWays’ project. The main differences occur in the manner that the command-and-control strategy is utilised. In Japan and Korea, the government ministries may outline the targets facilitating cooperation. However, they retain little control over private companies. On the other hand, the Chinese government has a more significant role in the economy and influence across the university sector, demonstrating closer alignment. The UKH2Mobility has outlined three stages for HFCVs and HRS rollout; seeding stage (2015-2020), accelerated ramp-up (2020-2025) and established market (2025-2030) (UKH2Mobility, 2016). The long-term goal of hydrogen is uncertain and largely depends on the strategy employed, i.e. moderate, optimistic etc. and the role hydrogen will play in the passenger vehicle sector, i.e. market share of HFCVs. Current emission targets in the UK aim to remove all petrol and diesel private vehicles from the road no later than 2050 (Committee on Climate Change, 2019). The end goal of hydrogen and its role in this sector will determine the magnitude of investment required by the government and private companies allowing all stakeholders to work towards the same goal. The following section encompasses the different mathematical approaches used by researchers to determine the hydrogen demand and the factors considered to achieve this.

2.5 An overview of the UK's case study and why it is appropriate

The UK was chosen as the case study in the current analysis for many reasons. First, the UK intends to reduce the net carbon account for the year 2050 by at least 100% than the 1990 baseline see P3.1 in section 3.2.2. The private sector will need to be fully decarbonised to achieve this objective unless other sectors contribute. Second, the UK is increasingly changing and improving current policies to set stringier and more ambitious targets to reduce GHGs and emissions as outlined in P3.2, P3.3, P3.4 (section 3.2.2), and P4.1 (section 4.2.2). It is essential to determine if current pledges of investment and work undertaken meet the requirement to honour the policies set by the UK's government. If not, what does the UK need to do to achieve its aims in decarbonising the passenger vehicle sector? Third, the UK produces approximately 26.9 TWh/year of hydrogen from approximately 15 sites whose capacities can be increased to the surplus of up to 3.5 TWh/ year and support early market adoption for transportation and other energy systems (Energy Research Partnership, 2016). What does this mean for the use of hydrogen as a transportation fuel? As stated previously, is the UK making sufficient progress or simply delaying the need to respond rapidly. Fourth, Shell and ITM Power have extended their agreement to deliver hydrogen refuelling to UK's customers, which will help to accelerate the introduction of hydrogen as a viable commercial fuel (ITM Power, 2019). Fifth, hydrogen and electricity have a perfect synergy to provide and store energy not only for the transport sector but for other sectors too. Sixth, both hydrogen and electricity can be produced from RES, thus reducing the UK's dependence on fossil fuels, and providing energy security. For these, and many other reasons, hydrogen is expected to play a key role in reaching the UK's transportation emission targets. Furthermore, the data required to consider the UK is readily available in literature, and government's official statistics (Almansoori and Shah, 2012; UKH2Mobility, 2013; Moreno-Benito et al., 2017; DfT, 2018).

2.6 Proposals selected from the literature

Three different proposals/case studies were selected from the literature to engage current projections for hydrogen demand. These were intended to analyse the model developed critically. The proposals consider the design of a potential HSC network in the UK from a pre-commercialised one to an established one each presenting various scenarios. The initial study used as a benchmark was carried out using data from the UKH2Mobility report (UKH2Mobility, 2013). The H2mobility group consists of directly involved stakeholders in the pre-commercialisation phase of introducing hydrogen in the UK. The report made projections for hydrogen from 2015-2030 in three five-year periods. Initially, smaller stations will be built to instigate the need for hydrogen and give vehicle manufacturers a platform to focus on HFCVs. As the network develops, it is expected that larger HRS will be built to accommodate the increase in demand – smaller stations will also be upgraded to increase the capacity. The selection of the UKH2Mobility is crucial as it reflects the ambitions and work proposed by the government in establishing a hydrogen infrastructure in the UK.

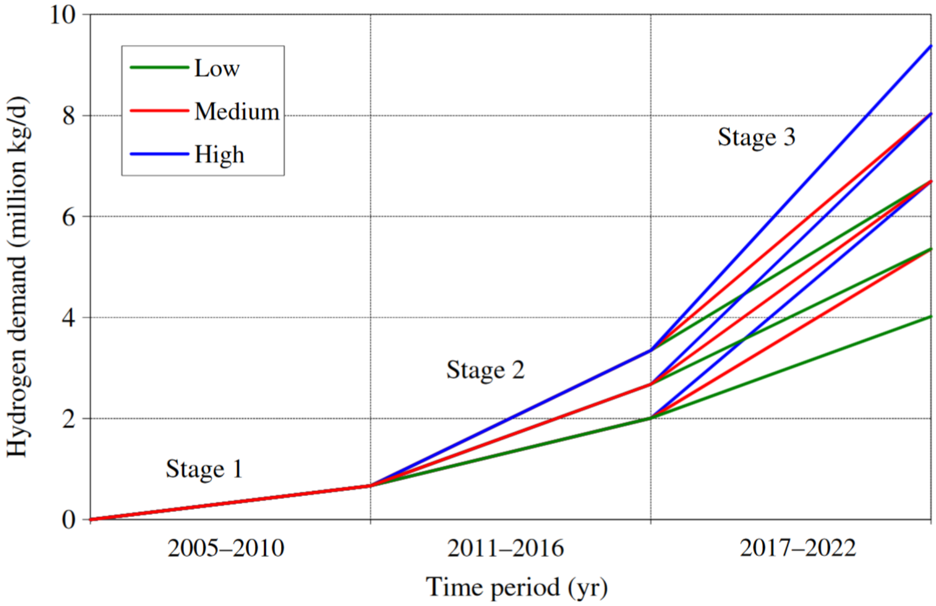


Figure 2. 3: Demand tree of scenarios adopted from (Almansoori and Shah, 2012).

The data and scenarios used by Almansoori and Shah were considered in the second proposal (Almansoori and Shah, 2012) because their work has been used extensively in modelling hydrogen for road transportation. The scenarios simulated are represented below in figure 2.3, representing the period 2005-2022. Here the demand for hydrogen was taken to be uncertain, and so therefore, 9 scenarios were assumed as demonstrated below. In the first stage, the demand for hydrogen was constant. In the second and third stages, the hydrogen demand was varied, giving several scenarios. Finally, the case study by Moreno-Benito et al. (2017) was considered to assess the current proposals in light with the UK's targets and current level of investments. Moreno-Benito et al. considered 2020-2070 for 50% market penetration of hydrogen with a consumption of 5000 tonnes of hydrogen/day solved using 5-year intervals. As a result, hydrogen is expected to achieve full penetration by 2120 (figure 2.4). There are few studies that have considered the UK as a backdrop for their models. As a result, limited studies and data is available. The abovementioned scenarios have complete data available and used extensively since.

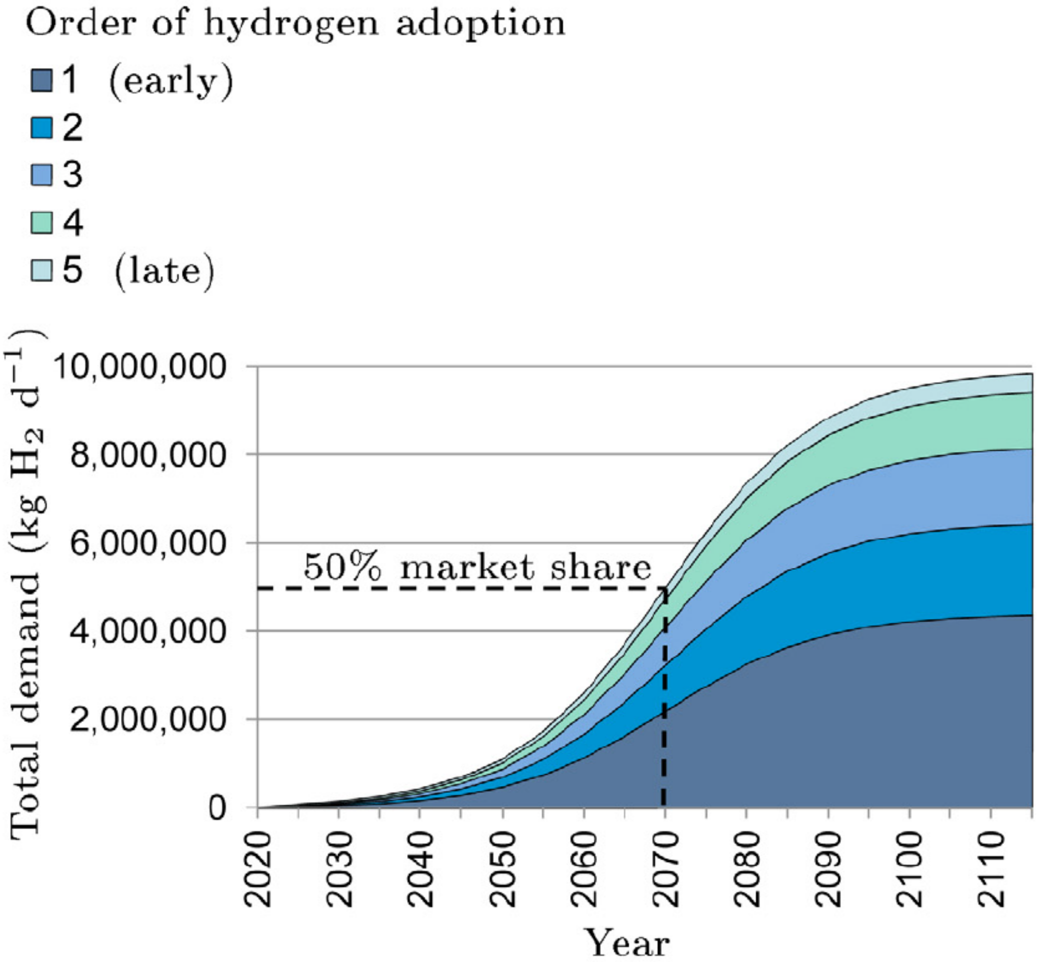


Figure 2. 4: Showing the market share of hydrogen adopted from (Moreno-Benito et al., 2017).

2.7 Research gap

In this thesis, the literature review firstly focused on the different models and scope of research undertaken for the transition to a hydrogen-based network. One of the key gaps identified in the literature was the approach used by researchers to analyse the introduction of hydrogen as a transportation fuel. The studies either considered a supply chain or two to determine the hydrogen demand required to support a particular scenario (Reuß et al., 2019; Obara and Li, 2020) or by considering a single node of the supply chain e.g., the hydrogen storage option (Seo et al., 2020). The studies for the UK are limited both in number and in terms of pre-selecting a supply chain focusing on a single or two options (Almansoori and Shah, 2012; Moreno-Benito et al., 2017). This is limited because all options are not investigated for each node of the supply chain.

Many studies have considered HSC within the local or national scale while determining the ideal configuration that best optimises the objective(s) of the model (Messaoudi et al., 2019; Obara and Li, 2020). Here, technical details are favoured by other factors considered exogenous such as the availability of resources. Due to the nature of the private vehicle fleet, multiple fuels are expected to meet the overall demand of the sector, and it is expected that the HRS network will be under-utilised for a period. Demand will vary, and operating efficiency of HRS must be considered (Mayer et al., 2019) to prevent long periods of under-utilisation and instances of over exploitation. Majority of the studies have focused on a particular supply chain or a particular node of the supply chain. The entire private fleet needs to be considered holistically to understand how different decisions and variable influence others.

The second aspect of the literature review was dedicated on examining the hydrogen infrastructure through the lens of hydrogen demand. The targeted market in this thesis is the transport sector considering HFCVs for the private vehicle sector. Hydrogen demand is an essential factor in designing the infrastructure in terms of size, and decisions made at different nodes. Hydrogen demand will also shape the HSC in terms of the number of stations, feedstock used to produce hydrogen, storage options and refuelling options used (Yoon et al., 2022). Most importantly, the magnitude of hydrogen demand will determine whether a centralised or decentralised approach is used (Seo et al., 2020). Further research is required to develop an understanding of the impact of hydrogen demand on decision variables in modelling and how the outcome will inform policies. Currently, the magnitude of demand relies on the decision metrices used by the researcher in terms of the scenario, vehicle efficiency, distance travelled etc. Considering the entire private fleet holistically extends the space to a macro level, this will allow the systematic elimination of unrealistic scenarios.

This is important because the future transport network will be multi-fuel based rather than conventional. Some of the limitations associated with current research is that they consider the introduction of a vehicle type into the market independently (Bae et al., 2020, 2021; Chu et al., 2022; Wickham et al., 2022), and secondly, they do not consider the impact of conventional vehicles and the push-back. The breadth of modelling types considered need to be expanded to encompass this behaviour. Further research is necessary to take the dynamical behaviour into account, and the inclusion of the LVM directly captures this behaviour. Current models in the literature consider the introduction of HBVs on their own, however any new vehicle introduced to the market will compete against current conventional vehicles. This is a limitation of current models because conventional technology is being improved, by improving efficiency and reducing emissions (ICCT, 2015). Therefore, it is expected to continue playing a significant role in the UK's private fleet. Further research is necessary to take the dynamical behaviour into account, and the inclusion of the LVM directly captures this behaviour.

Another gap lies in determining the criteria for the growth of HFCVs, which is multifarious as seen in the above section. In addition to this, the type of scenario depicted by the researcher, or the HSC under consideration also impacts the demand e.g. assuming a high penetration of HFCVs (Baufumé et al., 2013a). Researchers have also considered a number of scenarios by varying the penetration strategy of HFCVs (Baufumé et al., 2013b; Seo et al., 2020). Some studies have selected different scenarios based on penetration strategy for HFCVs i.e. pessimistic, moderate and optimistic (Almansoori and Shah, 2012; Liu et al., 2012; Talebian et al., 2019b). The penetration rate is an important metric in that the growth of hydrogen will be determined by many external factors. All these factors cannot be considered in the model without excessively complicating it. Research is required in utilising the penetration strategy as an exogenous factor.

The hydrogen demand projected is crucial for long-term planning of the UK's private vehicle fleet. The approach selected will largely influence the type of role hydrogen will play in this sector, i.e. a niche application fuel or a competitive mainstream one. Extrapolating from short-term aims to long-term ones will not always lead to sensible solutions, it is important to consider the entire passenger fleet holistically, considering UK's policies and current work to form a better understanding of its role. Table 2.2 summarises the key features of an ideal model that is assumed to represent the hydrogen uptake for the UK's private vehicle fleet, holistically. Currently, policies and investments have considered standalone HRS to initiate the implementation of a pre-commercialisation network of stations across strategic points across the country. Each of these stations will play an important role in terms of accessibility, the capacity of hydrogen and actual production.

In conclusion, based on the specification developed, there is a gap in the literature of a model representative of hydrogen uptake from a holistic viewpoint considering other fuels. Furthermore, the models discussed in the literature did not consider the impact of HFCVs on conventional vehicles. It was assumed that introducing HFCVs is independent of the conventional vehicle fleet when it is highly likely that stricter policies will quickly follow the successful penetration of alternative powertrains. It is clear from the literature that the hydrogen demand is instrumental in shaping the infrastructure; the scenarios, penetration rate, spatial and temporal data all contribute to the refuelling infrastructure and so, therefore, must be considered whether as exogenous or endogenous inputs.

Table 2. 2: Specification of an ideal model

Specification	**Corresponding model feature**
Estimation of the hydrogen demand	To capture the hydrogen demand. How is it derived? Justification of the scenarios or selection of market share of hydrogen fuel.
Economic analysis of introducing HFCVs	To strike a hydrogen demand/supply balance Growth rate of HFCVs Impact of alternative fuels/competitors Accountability of regulations on UK's emissions reduction targets.
Temporal aspect of HFCVs	Alignment of hydrogen introduction alongside the period outlined in regulations to reduce GHG emissions.
HRS network	The number, type of refuelling stations considered. Operating efficiency of the stations.
Hydrogen penetration Strategy	What type of strategy will be employed? Pessimistic, moderate, or optimistic?

Chapter 3: First-order growth model of the UK's passenger vehicle fleet

3.1 Introduction

This chapter firstly introduces the overall methodology of the thesis that underpins the research undertaken. A brief overview is given on the classical LVM model before providing a detailed explanation of the first-order growth model concept. This includes the model description to explain the first-order growth model including the policies, and assumptions. The implementation of the growth model for the UK's passenger fleet is described and demonstrated based on this analysis. The results and validation are also provided before discussion and insights. Finally, limitations of the first-order model are presented alongside the need to develop the second-order model.

3.1.1 Overall Methodology

The research in this thesis uses a dynamic modelling approach to develop a realistic model of evolution of the private vehicle fleet in the UK to inform policy makers. The implication from this is that the model must be comprehensible, informative and encompasses the fleet composition for polities to be drafted. A lack of historical data of hydrogen fuel cell vehicles is considered as a limitation in using forecasting models (Park et al., 2011a). In this chapter, the economic growth model developed is driven by the data from conventional vehicles to overcome this limitation. Furthermore, the use of dynamical systems to model the HSC opens possibilities of integrating various powerful mathematical tools. Since other vehicle types such as electric vehicles (EVs), non-fuel cell hybrids will also play a role in the private vehicle market, and new vehicles will compete with conventional vehicles makes the representation of mutual interaction necessary, for this reason the Lotka-Volterra Model (LVM) is selected and presented below. The classical predator-prey system was first considered by Lotka in 1920 modelling undamped oscillations for chemical reactions and then later by Volterra to predator-prey interactions (Beals et al., 1999; Hoppensteadt, 2006). To represent the private vehicle fleet more accurately, the predator-prey equations will be modified in chapter 4 using economic growth principles. Growth curve modelling is a universal term used in different contexts encompassing various statistical models to map the growth of a product.

3.1.2 Lotka-Volterra Model

The LVM is based on the growth model exploring interactions between two or more diverse competitors (Chiang, 2012; Wang and Wang, 2016a). The LVM is composed of a pair of first order autonomous ordinary differential equations (ODE) that describe the predator-prey dynamics in their simplest case (Beals et al., 1999). The equations representing the LVM are given below (Hoppensteadt, 2006):

$$\dot{x}_1 = (a - bx_2)x_1$$
$$\dot{x}_2 = (rx_1 - d)x_2 \qquad \text{Equation 3. 1}$$

The parameter a represents the growth rate of competitor x_1 (prey) in the absence of interaction with competitor x_2 (predators). Prey numbers are diminished by these interactions: the per capita growth rate decreases (here linearly) with increasing x_2, possibly becoming negative. The parameter b measures the impact of predation on $\dot{x}_1/x_1$ i.e. the attack rate. The parameter d is the death (or emigration) rate of species x_2 in the absence of interaction with species x_1 or the growth rate. The term rx_1 denotes the net rate growth (or immigration) of the predator population in response to the size of the prey population.

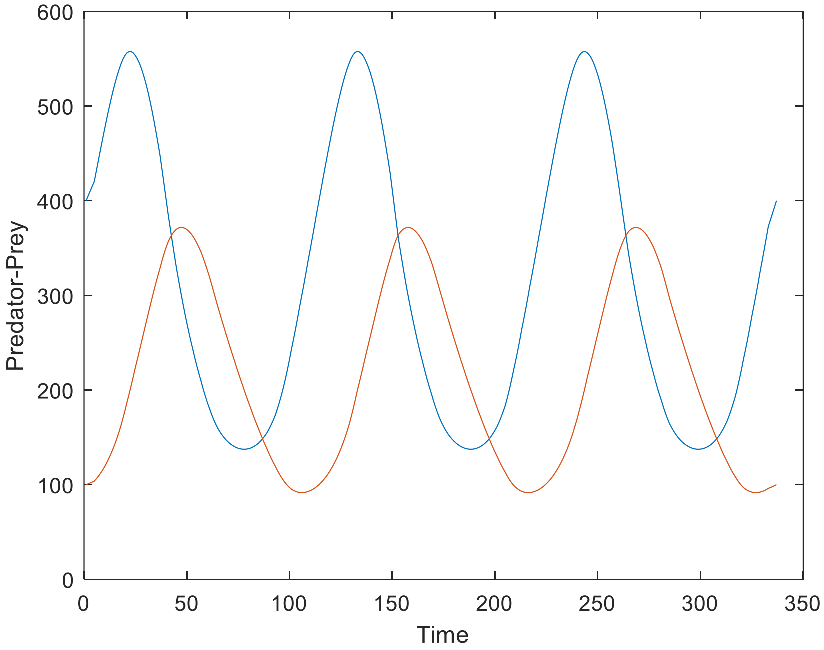


Figure 3. 1: Time series plot of the classical predator-prey model showing the evolution of 100 predators (red) and 400 prey (blue).

The LVM (see fig 3.1) is characterised by oscillations in the population size of both predator and prey with a lag in the oscillation peak of the predator to the prey. This is both suitable and explains the dynamic phenomena in population dynamics (Peckarsky et al., 2008; Thierry et al., 2015). However, such an oscillatory behaviour is not realistic for the evolution of conventional and hydrogen-based vehicles fleets. This characteristic must be limited to reflect the growth and decay of the private vehicle fleet. Alternative vehicles are expected to displace conventional vehicles following the same trajectory. The growth of conventional vehicles will decline due to depletion of fossil fuel, environmental concerns, and the development of more efficient technology. So, therefore, it is necessary to modify the Lotka-Volterra equations to represent the UK's road transportation environment.

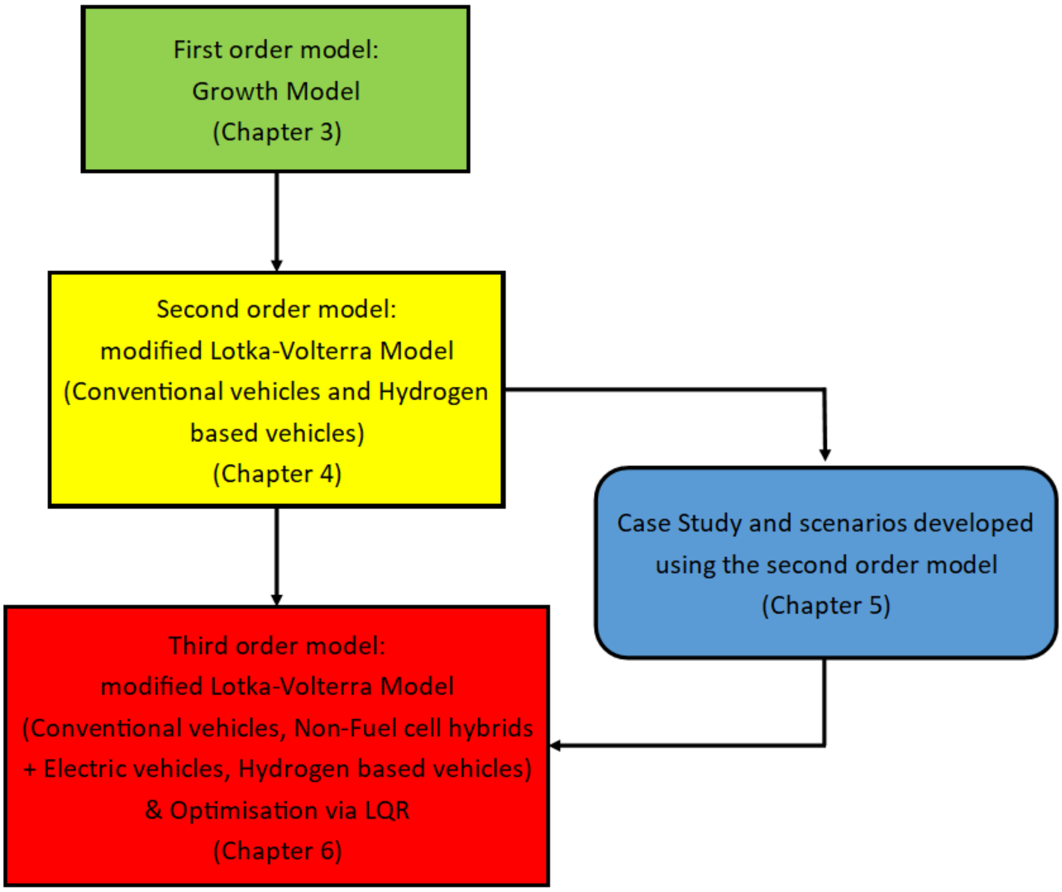


Figure 3. 2: Overview of the methodology

Figure 3.2 summarises the overall methodology used in this thesis. In this chapter, the first-order growth model is developed to represent the growth of the fleet. In chapter 4, the LVM is modified to encompass more realistic dynamics derived from the first-order model. The modified LVM is a second-order model consisting of 1 predator and 1 prey. Chapter 5 represents the case study and scenarios developed from the second-order model to inform the third-order model developed in chapter 6. The third-order model consists of three variations in terms of the predators and prey as outlined in figure 6.1. The LVM has been extended in many other studies (He et al., 2012; Hsu et al., 2015; Aybar et al., 2018) to capture the relationship or interaction between multiple preys or predators. The current private vehicle fleet constitutes of multiple vehicle types, and to meet future demand, it is increasingly likely that the fuel consumed will be more diverse making it necessary to extend the model to take more competitors into account.

3.2 First-order growth model concept

3.2.1 Determination of the boundaries of the hydrogen demand

One of the gaps outlined in the literature review is a lack of an in-depth analysis of the hydrogen demand from a holistic viewpoint. Current studies have used various approaches and variables to determine the hydrogen demand for a specified supply chain (SC) before extrapolating it to represent the region or country. The hydrogen demand is a defining factor for investing in the hydrogen infrastructure for the private vehicle market in the UK. This research will consider the private vehicle market holistically to determine the hydrogen demand by assuming the displacement of the entire fleet by Hydrogen - based vehicles (HBVs) as the upper limit to achieve decarbonisation.

3.2.2 Policies considered in this chapter

The following policies were considered when developing the model, and to determine relevant assumptions. Governmental policies and incentives are vital in promoting hydrogen as a transportation fuel and for consumers to accept HBVs (Maryam, 2017; Chu et al., 2022).

Policy 1 (P3.1): The net UK carbon account for the year 2050 is at least 100% lower than the 1990 baseline. The 1990 baseline refers to the aggregate amount of net UK emissions of $C0_2$ for that year, and the net UK emissions of each of the other targeted GHGs for the year that is the base year for that gas (legislation.gov.uk, 2019a).

Policy 2 (P3.2): The UK government announced in 2017 that it will end the sale of all new conventional petrol and diesel cars and vans by 2040 (GOV.UK, 2017b).

Policy 3 (P3.3): PM Theresa May in 2018 pledged that all new cars and vans will effectively be ‘zero emissions by 2040’ (GOV.UK, 2018a).

Policy 4 (P3.4): The Scottish government has made a commitment to use Ultra-Low emission vehicles (ULEVs) and to phase out the need to buy new petrol and diesel cars or vans by 2032, ahead of the UK Government's 2040 target (Committee on Climate Change, 2019; GOV.Scot, 2019).

3.2.3 Assumptions undertaken for the first-order model

The growth model was developed taking the following assumptions into account:

Assumption 1 (A3.1): The first-order model will cover a period of 100 years; the growth of conventional vehicles will be determined from 1960-2010 and forecast for the following 50 years taking P3.1 into consideration.

Assumption 2 (A3.2): The growth model only considers road passenger vehicles. Other forms of vehicles such as vans is beyond the scope of this thesis. This is based on P3.2, P3.3 and P3.4, where conventional vehicles will be phased out from the sector.

Assumption 3 (A3.3): The growth rate of the private vehicle fleet is expected to remain constant in the future, following the current trend of a 5% growth rate. The general trend suggests that vehicles will continue to increase (DfT, 2019; Leibling, 2008a).

Assumption 4 (A3.4): It is assumed that conventional vehicles have peaked and are at a decline. This is coherent with announcements made by the government to ban petrol and diesel cars and vans by 2040 (P3.2) (GOV.UK, 2017a).

Assumption 5 (A3.5): New petrol and diesel vehicles manufactured are classified as mild or other hybrid as hybrid technology is integrated e.g. regenerative braking (Cobb, 2014).

Assumption 6 (A3.6): The wasted mass of the total mass of fuel used in a vehicle per year is neglected.

Assumption 7 (A3.7): The mass of fuel is calculated by the number of vehicles that can be supported, meeting the statistics of road vehicles in the UK.

Passenger vehicles represent majority of the vehicles on UK's roads at approximately 30 million in 2018 and responsible for bulk of the emissions by road vehicles (Leibling, 2008a; GOV.UK, 2019). The growth of private vehicle is expected to continue a similar trajectory until public transport infrastructure is developed further. Agnolucci et al (2013) selected a scenario where HBVs continued penetrating the market as historical analogies. The impact of AFVs on conventional vehicles and vice versa is critical in understanding how soon the UK is able to decarbonise the private vehicles fleet, especially with minimal infrastructure. The LVM captures the mutual interaction between competitors making it an ideal methodology to assess the impact of different policies.

3.2.4 Governing Equations of the modified growth model

Historically, the growth of conventional vehicles has been modelled as linear, (Leibling, 2008a) suggesting that the fleet will continue to grow without a cap. This, however, is incorrect because the fleet growth will decline due to several factors. This includes the availability of fuel, alongside the implementation of policies, and emission reductions in line with P3.1, P3.2, P3.3, and P3.4. Due to the nature of conventional fuel, i.e. it is non-renewable, it is expected that this will be the end of the traditional ICEVs and will not see a resurgence in the vehicle market. In saying this, the transient growth can be seen in a first approximation, as linear in first order models.

A first-order equation has been developed to map the growth of conventional vehicles as stated in A3.1. The total mass of fuel $\dot{m}_t$ used by the fleet of vehicles per year is calculated by combining the rate of mass being consumed, $\dot{m}$, with the mass wasted $\dot{m}_w$ (Equation 3.2). The growth of conventional vehicles is expected to have reached a saturation point with the manufacture of alternative vehicles and will decline after that.

$$\dot{\boldsymbol{m}}_t = \dot{\boldsymbol{m}} + \dot{\boldsymbol{m}}_w \qquad \text{Equation 3. 2}$$

A3.6 is assumed here to simplify the calculations by equating the mass wasted to zero resulting in $m_t = m$. The total mass of fuel consumed in a year is equal to the number of vehicles (N_v) multiplied by the mass of the conventional fuel consumed per vehicle per year (m_i). Equation 3.2 can be applied to any fleet, and for conventional (ICEV) vehicles, the total mass (m) would be the mass of petrol used per year, while for hydrogen, it would be the mass of hydrogen being used per year.

$$\boldsymbol{m} = \boldsymbol{N}_v \boldsymbol{m}_i \qquad \text{Equation 3. 3}$$

Differentiating equation 3.3 gives us equation 3.4. $\dot{m}$ represents the rate of total mass consumed in a year.

$$\boldsymbol{\dot{m} = \dot{N}_v m_i + \dot{m}_i N_v} \qquad \text{Equation 3. 4}$$

The resulting equation is then rearranged to get the number of vehicles rate.

$$\boldsymbol{\dot{N}_v = -\frac{\dot{m}_i N_v}{m_i} + \frac{\dot{m}}{m_i}} \qquad \text{Equation 3. 5}$$

Since this is a first-order system, then $\frac{m_i}{\dot{m}_i}$ is equal to the constant τ, which is assumed to be constant and the parameter characterising the response to a step input of a first-order system.

$$\boldsymbol{\alpha = \frac{\dot{m}_i}{m_i} = \frac{1}{\tau}} \qquad \text{Equation 3. 6}$$

The second term in equation 3.5 is represented by $\boldsymbol{\mu}$ (equation 3.7).

$$\boldsymbol{\mu = \frac{\dot{m}}{m_i}} \qquad \text{Equation 3. 7}$$

Here, the quantity of $\boldsymbol{\mu}$ is the mass of fuel used annually divided by the mass of fuel consumed by a vehicle. This, in turn, corresponds to the maximum number of new cars that can be absorbed yearly by the supply chain of fuel. Rewriting equation 3.5, we get equation 3.8, representing the growth model.

$$\boldsymbol{\dot{N}_v = -\alpha N_v + \mu} \qquad \text{Equation 3. 8}$$

The amount of fuel consumed by a vehicle annually is positive ($m_i > 0$) and this can be approximated by a constant so long as there is no breakthrough in technology. This implies that the growth rate is negative (i.e. decay) and is being driven by the resources, and in the absence of resources or fuel, the number of vehicles will reduce to zero. So, therefore, the inclusion of a fuel term mitigates this dynamic, and the available fuel acting as the resource will increase the number of vehicles.

If this is not the case, then it is expected that $d(m_i) < 0$ because new cars are more fuel efficient than old cars. It means that $\alpha < 0$, and $-\alpha > 0$, in other words $\frac{d(m_i)}{dt} > 0$ implying that the supply chain is growing. This also means that $\frac{dN_v}{dt}$ will always be positive, it will only stop growing if $\frac{dm}{dt} = 0$, and $\frac{dm_i}{dt} = 0$.

Assuming the amount of fuel a vehicle consumes is constant, $\dot{m}_i$, and that the fuel consumption per year will reach an optimum value. Taking the limit, the number of vehicles will then reach a plateau as well:

$$\lim_{t\to\infty} N_v = \frac{\dot{m}}{\dot{m}_i}$$

This value depends exclusively on the fuel resources available for consumption per year, divided by the individual car consumption, i.e. the number of cars that the supply chain can support. It is a fundamental difference with a standard growth model that diverges. The growth model is stabilised.

The model can represent the growth of conventional vehicles for the UK and other countries using the corresponding data. The effectiveness of the first-order model to predict the growth of conventional vehicles was evaluated by considering the number of carparc projections in the UK to select appropriate parameters. AFVs were not included here in par with A3.4 as new vehicles are classified as hybrids due to the technologies being used, e.g. regenerative braking. This data demonstrated a 5% decay rate for the UK (Leibling, 2008). Figure 3.3 shows the block diagram of the growth model in Simulink.

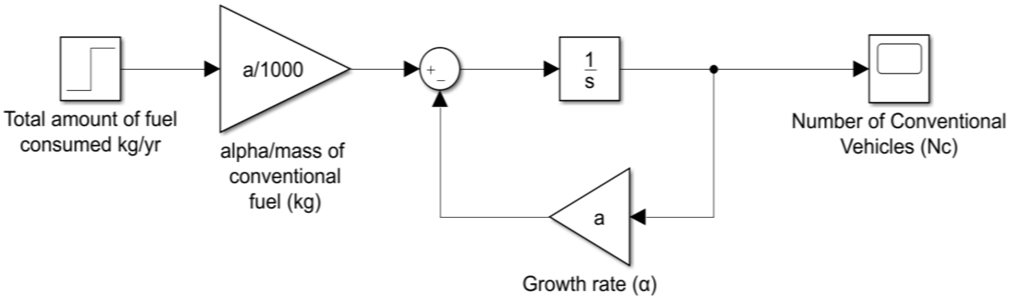


Figure 3. 3: Growth model represented in Simulink block diagram.

The total fuel consumed per year is the step input in par with A3.7, with "α" being the growth rate of conventional vehicles in accordance with A3.2, and A3.3. The model was simulated for the UK to see if the first-order growth model gave plausible results. The values representing the parameters used in the simulation are summarised in table 3.1. The parameters were selected based on the model fit using the data available from literature, e.g. the fuel input data was calculated by the number of vehicles using MATLAB Simulink. Official statistics for the UK (GOV.UK, 2019) and those from the RAC Foundation (Leibling, 2008) will be considered to validate the model and parameters selected.

Table 3. 1: Parametric constraints used in the growth model for the UK, and for validation CA, and Japan.

Parameter	Estimated Value	Reference	Location
Fuel Input	3.2e10 kg	(Leibling, 2008a)	UK
Growth rate	0.05		
Fuel Input	1.5e10 kg	(Statista, 2017)	California
Growth rate	0.06		
Fuel Input	6.09e10 kg	(JAMA, INC, 2016)	Japan
Growth rate	0.09		

The growth model was further extended to model the growth of road vehicles in California and Japan. Japan, and CA were selected for their substantial work on integrating hydrogen and alternative fuel into their transportation fleets. Cumulative sales of HBVs from 2015-2018 in CA have increased steadily, influenced by having sufficient infrastructure in place prior to market introduction (CaFCP, 2018b). Japan is the first country in the world to open 100 HRS for road transportation (Kyodo News, 2018) ahead of CA. This is significant because of the size of Japan (377,972 km^2), with a population of 126.8 million in 2017, in comparison to CA (423,970 km^2) that had a population of 39.54 million in 2017 (THE WORLD BANK, n.d.). Furthermore, the 100 HRS provides coverage in Japan geographically, which is not the case in the USA. The UK is trying to establish a similar idea to Japan with HRS established across key motorways and larger cities (UKH2Mobility, 2013). As the demand for hydrogen grows, Japan will require to open larger stations as and when required.

3.3 Results obtained by modelling the growth of conventional vehicles

3.3.1 Model Validation

The first-order growth model developed was simulated in MATLAB Simulink, and figure 3.3 shows the growth of the UK's passenger vehicle fleet. The number of vehicles projected by the growth graph is just above 30 million (figure 3.3) in 2017 (Leibling, 2008a; DfT, 2018, 2019). The parameters shown in table 3.1 and A3.1 show the amount of conventional fuel consumed in the UK, Japan, and CA alongside their respected growth rates. This is significant since the amount of fuel consumed was extrapolated from the number of private vehicles on the road (Leibling, 2008a; DfT, 2019). It is also a means of validation for the model. So, if the model projects the number of expected vehicles from the quantity of fuel consumed, then the parameters selected are correct and suitable.

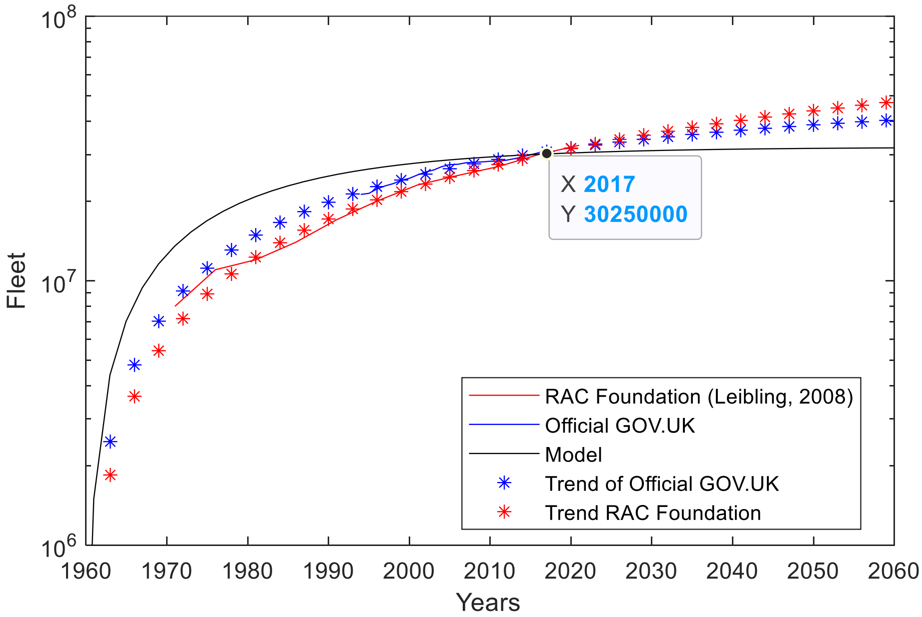


Figure 3. 4:Comparison between official data from GOV.UK, RAC Foundation and the model

In addition to this, the sector has seen 5% growth every year for the last decade (Statistica, 2016), and is expected to continue as hypothesised by A3.3. Figure 3.3 also demonstrates incremental growth beyond 2015/2020 for conventional vehicles.

The two sources covered different year periods in terms of the data used, while data covering the entire 50 years period is not available. A logarithmic best fit was used to demonstrate the general trend covering from 1960 and projecting to 2060. Renormalisation was used to overcome the scale invariance between the different data sets, allowing comparison between the forecasts. The model demonstrates a steeper growth than GOV.UK and Leibling's data before reaching a plateau.

Furthermore, the trend lines also forecast that growth will continue along the same trajectory. This was demonstrated by the percentage difference calculated; the Leibling plot and model percentage difference is 0.611% and between the model and GOV.UK it is 0.749% using the following formula:

$$\boldsymbol{Percentage\ error} = \left(\frac{\boldsymbol{data - model}}{\boldsymbol{model}}\right) \times \mathbf{100} \qquad \text{Equation 3. 9}$$

California (CA) and Japan were selected as different geographic areas to further test the developed growth model. Both CA and Japan lead the field in utilising hydrogen as a transport fuel or energy carrier (CaFCP, 2018; JAMA, INC, 2016). Japan saw a growth of 9% up to 2016, whereas CA's road vehicles saw a growth of 6% until 2017. The growth rates representing CA and Japan were used in table 3.2. Here, the model was able to represent the number of vehicles closely to those expected (see figure 3.4). The percentage difference in actual data for 2015 and the simulated model for Japan was 0.66%, and the difference between the actual CA figures and those from the model is 0.28%.

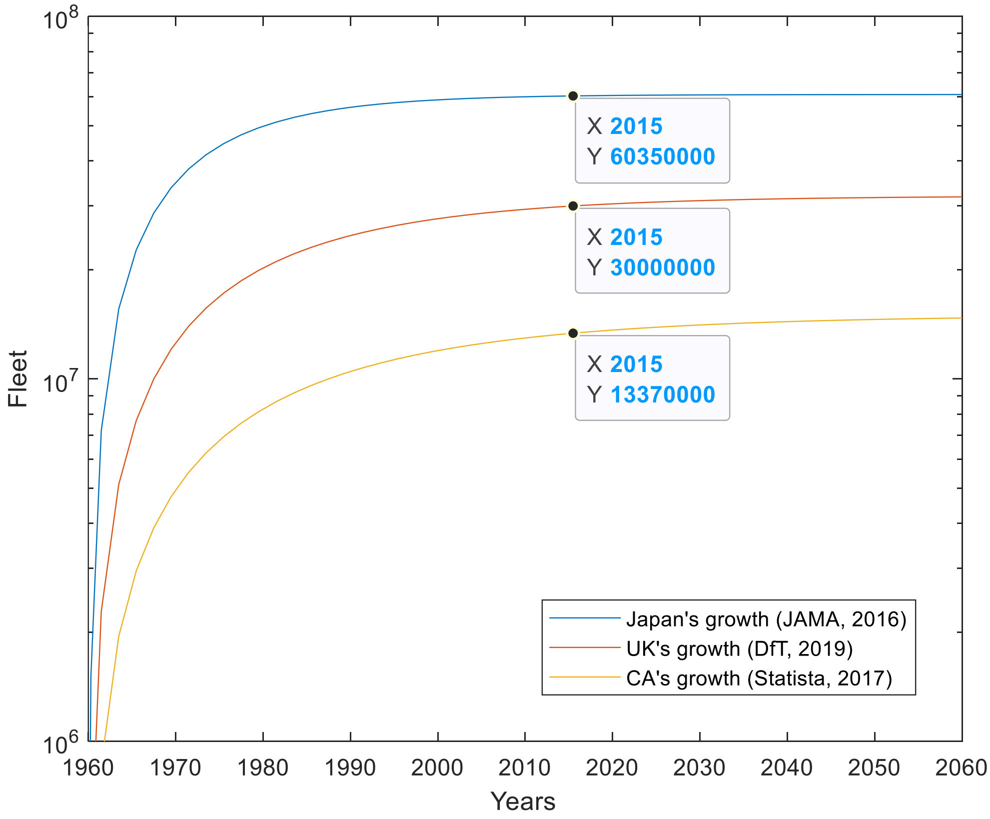


Figure 3. 5: Growth of Japan, UK, and CA from the fuel consumed.

The growth model allows the passenger vehicle sector to be considered in a holistic viewpoint, rather than HSCs, as in the case of other studies. This will help determine the proportion of different vehicle types according to funding, government policies on the climate and transport and recent investment by various stakeholders. The growth model is suitable to be incorporated into the LVM to represent the UK's passenger vehicle environment by overcoming its limitations.

3.3.2 Discussion and Insights

This chapter proposed a first-order growth model to produce a realistic reflection of the growth induced by the UK's private vehicle fleet. The implemented model was used to assess the potential space available for HBVs. The model considers an alternative means of determining the hydrogen demand, simplifying the methods currently used as described in the literature review (Seo et al., 2020; Tlili et al., 2020; Liu et al., 2012). Usually, the hydrogen demand is proposed by the researcher according to a particular HSC (Almansoori and Shah, 2012). However, in this case, the entire fleet is considered holistically, which leads to more varied scenarios and the elimination of highly unrealistic ones. Additionally, the growth model enables the inclusion of the temporal aspect of the forecast model using SIMULINK. However, this is often portrayed in the literature by encompassing the multi-period aspect (De-León Almaraz et al., 2015a; Almansoori and Shah, 2012). Inclusion of the temporal aspect is important to envisage the decarbonisation of the passenger vehicle fleet by 2050 according to current policies.

Generally, there is a lack of historical data concerning forecasting new technologies, so alternative technologies are often considered to predict the behaviour of new technologies to the market. Data concerning the number of private vehicles in the UK over this period is also incomplete. Official UK statistics start to document the number of private vehicles and the different types from 1994 (GOV.UK, 2019). Since the official statistics cover only a partial section of the period under consideration, those documented by the RAC foundation starting from 1971 were also used to validate the data (Leibling, 2008). In this case, it was not essential to have complete data, as some of the parameters were determined from the model using the current number of vehicles documented. For instance, the model was used to determine the correct number of vehicles supported by the amount of fuel consumed. The amount of fuel consumed in a year in the UK was determined from the number of private vehicles in the UK using official data for 2018 (GOV.UK, 2019).

Figure 3.3 depicts the growth of the UK's conventional vehicle fleet using the official data from GOV.UK, RAC Foundation and the model. The model demonstrated a steeper growth than both the official data, and RAC Foundation, with a difference of 0.749% between the model and GOV.UK, whereas the difference between the model and RAC Foundation was 0.611% using percentage error between the curves. The percentage error could have been reduced further by manipulating the parameters further using trial and error. However, the point of interest here was where the three curves converged at 30.25 million vehicles in 2017. Since the amount of fuel used was able to support 30 million vehicles, the model levelled out. The trend line for both the official data and RAC foundation continues the 5% growth trajectory. The purpose here was to determine the parameters of the model rather than producing a 100% accurate replica of the market. The trends of the two sources follow that of the model, suggesting that both the model and its parameters are sensible and able to predict the growth of conventional vehicles.

The modelling of conventional vehicles was important to limit the oscillations projected by the general predator-prey model. The conventional behaviour of the generalised LVM must be limited in this application because conventional vehicles will not see a resurgence after declining due to the limited supply of fossil fuels and their corresponding environmental impacts. Since AFVs are competitors to conventional vehicles, the number of EVs and hybrids were not included alongside the number of conventional vehicles in the model, according to A3.5. The simulation graph, however, projects growth in the sector based on the 5% growth rate. The number of road passenger vehicles is expected to increase. New vehicles are now incorporated with hybrid technology such as stop-start, regen braking, and so classified as mild hybrids. So growth in the passenger sector is essentially hybrid vehicles dictated by the ban on the sale of petrol and diesel-based vehicles being rolled out by 2040 (GOV.UK, 2017b).

The model was further validated by using data for different regions to determine if the number of vehicles can be determined using the growth rate and fuel input. Figure 3.4 depicts the growth of conventional vehicles in Japan and CA alongside the UK. The growth rate of 7.2% was used for Japan and 6% for CA. Here, the model was able to represent the number of vehicles closely to those expected (see figure 3.4). The growth model demonstrated that the model produced plausible results when the passenger vehicle fleets of alternative countries were simulated. This suggests that given the correct or suitable growth rate, the introduction of alternative vehicles using the LVM will also be accurate. This is important because the generic predator-prey model follows a growth and decay pattern. Whereas, in conventional vehicles, we do not expect conventional vehicles to make a comeback in 50 to 100 years due to the lack of fossil fuels.

3.3.3 Limitations and transition to the second-order model

The purpose of this chapter was to determine the growth rate of HBVs by extrapolating the growth of conventional passenger vehicles in the UK across the last 50 years and projecting future growth. If the UK strives to achieve its target of 100% reduction in emissions by 2050 with respect to 1990 levels, then the transportation sector must be decarbonised over the same period. The first-order growth model represents the growth of conventional vehicles in the UK, allowing the space available for AFVs to be modelled. The model was validated by using the official UK data (GOV.UK, 2019) and the RAC Foundation (Leibling, 2008a). The model is suitable to be integrated into the LVM to assess the impact of introducing alternative vehicles.

The growth model looks at the passenger vehicle sector in a holistic viewpoint by taking the amount of fuel consumed in a year. The model does not take other factors into account, such as social influence, finance, number of vehicles per household (Dayhim et al., 2014) etc. The need to take these factors into account was overcome by using the carparc data for the number of vehicles in the UK, rather than estimating the number of cars per household. Some households may have more than one vehicle, and others none.

Simply developing the growth model is not adequate on its own in determining the outlook of the UK's passenger vehicle sector because only conventional vehicles were considered. Further growth of the sector will see an increase in AFVs, such as hybrids, and so their role must be considered independently to conventional vehicles. The input of AFVs is important in assessing what the UK's passenger vehicle sector will look like in the near to long term future. Will the sector continue to grow at the projected 5% growth rate? Or will conventional vehicles be replaced by mild hybrids? Or will EVs and HBVs play a much greater role? Instead of combining the number of AFVs with conventional vehicles, it is important to see the impact that AFVs will have on conventional vehicles and vice versa. By incorporating the growth model with the predator – prey model, the AFVs can be modelled as the predator acting independently of conventional vehicles. This will help realise the impact of AFVs on conventional vehicles while taking future growth into account and the current number of vehicles.

3.4 Conclusion

This chapter takes the growth of conventional passenger vehicles in the UK to gauge the space available for AFVs if decarbonisation is to be achieved by 2050. AFVs were modelled on their own to demonstrate the impact of introducing them into the sector. The growth model was used to represent conventional vehicles in this case, which will represent the prey in the second-order model. AFVs such as EVs and HBVs will be modelled separately as the predators also using the growth model.

The results of the first-order model show the following:

(1) Parameters outlined in table 3.2 are suitable to determine the growth of conventional vehicles in the UK utilising the first-order growth model.
(2) The growth model limited the behaviour of the predator-prey model, making it suitable for the application of introducing AFVs into the UK's private vehicle fleet.
(3) The growth model has reduced the number of constraints and factors that alternative models have considered, such as household income, number of vehicles per household.
(4) The growth model allows the passenger vehicle sector to be considered in a holistic viewpoint, rather than HSCs as in other studies.
(5) The growth model demonstrated that the model produced plausible results when the passenger vehicle fleets of alternative countries were simulated. It is suitable to be incorporated into the LVM.

Chapter 4: Second-order Lotka-Volterra Model

4.1 Introduction

In this chapter, the second-order predator-prey model for the UK's passenger vehicle sector is described in detail. This is a dynamic system based on Lotka-Volterra concepts, which assesses the interactions of two interacting technologies. In this instance, the introduction of hydrogen as a transportation fuel in the current conventional fuel dominant sector. The application of LVM has been used widely across disciplines as demonstrated in the following studies (Zu et al., 2015; Waters et al., 2015; Thierry et al., 2015; Marasco et al., 2016). One of the characteristics of the LVM is the capture of mutual interaction between two competing species or technologies showing growth and decay in response to the growth or decay of the other. In this case, conventional vehicles are expected to reduce in number and eventually taken off the road, but not re-introduced. The growth model developed in chapter 3 is incorporated here to modify the Lotka-Volterra equations to limit and represent the UK's road transportation environment. This allows the growth of conventional vehicles represented before introducing HBVs giving a more realistic environment in terms of the number of conventional vehicles on the road. The growth model is also important to assess the passenger vehicle fleet holistically by giving a sense of the space available.

The chapter firstly presents the second-order Lotka-Volterra Model, its description, policies, assumptions, governing equations, model simulation, and model validation. This is followed by the results in the following order: modelling and evaluating the plausibility of the second-order model, comparison of hydrogen refuelling stations, number of vehicles supported by different station types, and the case of whether investing in hydrogen fuel cell vehicles will be more advantageous than hydrogen-based range-extenders. The analysis is presented, followed the conclusions and the chapter summary.

4.2 Second order Lotka-Volterra Model

In this study, the second-order model was derived to model the interaction resulting from introducing alternative fuel vehicles (AFVs) into the conventional vehicle dominated market. This model extends the first order model by introducing the predator-prey concepts based on LVM. This model is useful in describing the interactions between conventional vehicles and any other AFV and capturing the mutual interaction element of the LVM as mentioned above.

4.2.2 Policies

Policies shape and define the way both consumers and stakeholders make their choices in developing products and using various services. It is essential to consider latest policies that will drive the future of the passenger vehicle fleet. The following policy is also considered as well as those outlined in section 3.2.2.

Policy 1 (P4.1): In order to ensure all petrol and diesel cars leave the fleet by 2050, all non-zero emission vehicles sold before 2035 could be certified for use on UK roads no later than 2050 (average lifetime of a vehicle operating on UK roads is 14 years) (Committee on Climate Change, 2019).

Policy 2 (P4.2): The UK has pledged to end the sale of new petrol and diesel cars by 2030 (DfT, 2020).

These policies are important to note in that petrol and diesel cars will be removed from the road in 2050 towards the end of the lifecycle.

4.2.3 Assumptions

This section explains the assumptions made for the second-order LVM:

Assumption 1 (A4.1): Conventional vehicles assume only the role of prey and do not predate on the other actor(s) as according to P4.1 and P4.2.

Assumption 2 (A4.2): The predator will always be an AFV (EV, hybrids etc.) for the same reasoning as A4.1.

Assumption 3 (A4.3): The second-order model will only have 1 predator- 1 prey relationship, this is following the classic predator-prey scenario (Peckarsky et al., 2008).

Assumption 4 (A4.4): The attack rate is varied for different predators depending on accumulative sales from official statistics (DfT, 2018).

Assumption 5 (A4.5): The approximate lifetime of a vehicle is not considered in the model. It is assumed that the vehicle replaced will be removed at the end of its life cycle according to P4.1.

Assumption 6 (A4.6): HBVs will be assumed to operate at 90% efficiency of the infrastructure's capacity. It is highly unlikely that HRS will operate at maximum capacity, and initially will probably operate below 25%. 90% was selected to visualise a future where HBVs are becoming popular and efficiency losses of HRS are minimised.

Assumption 7 (A4.7): HBVs will be refuelled once a week to calculate the amount of fuel consumed per year.

New cars are classified as hybrids depending on their level of hybridisation (Cobb, 2014). The number of conventional vehicles will not increase from current levels and so will not displace any AFVs.

4.2.4 Governing Equations

The predator-prey interaction consists of a pair of first order autonomous ordinary differential equations (ODE) as follows (Sharov, 1996) according to A4.3, and in this case were modified to encompass μ term. This term reflects the amount of conventional consumed by the fleet over a year.

$$\dot{x}_1 = x_1(-a + bx_2) + \mu_1 \qquad \text{Equation 4. 1}$$

x_1 is the number of ICEVs assuming the role of the prey as outlined in A4.1, x_2 is the number of HBVs (or AFV) assuming the role of predator as outlined in A4.2, a is the growth of conventional vehicles (ICEVs) i.e. rate of increase per unit time, b is the coefficient of predation rate (attack rate) of ICEVs to HBVs, and μ_1 represents the total amount of diesel and petrol in kg consumed by the entire country's fleet per year. Equation 4.3 represents the second equation of the ordinary differential equations with the additional μ_2 term representing the quantity of hydrogen fuel consumed by the fleet of HBVs.

$$\dot{x}_2 = x_2(-cx_1 - d) + \mu_2 \qquad \text{Equation 4. 2}$$

Here, c represents the efficiency of AFVs (i.e. the conversion rate of ICEVs into AFVs), d represents the growth of AFVs (per mass of hydrogen consumed per vehicle per year), and finally μ_2 represents the total amount of alternative fuel in kg consumed by the country's entire fleet per year. According to the LVM, if AFVs are equal to 0, so in other words, $x_2(t) = 0$, then the number of ICEVs is expected to grow exponentially by $\dot{x}_1 = aN$. The equations of LVM have been modified to include the growth model developed in chapter 3 to stabilise the growth.

4.2.5 Model Simulation

The second-order model presented in the above section was used to evaluate the effectiveness of introducing HBVs into the current vehicle market structure. Since the second order model considers the relationship between two interacting vehicle types, different predators were considered to evaluate the effectiveness of the model for e.g. ICEVs v HFCVs, ICEVs v HFC-RE, ICEVs v Hybrids non-FC + EVs. However, only the results from HFCVs and HFC-REs are presented here. The purpose here is to assess the plausibility of the model and its effectiveness in capturing the interaction of a new technology in an established sector. The following table represents the values of various parameters used in the Simulation. The parameters a, b, c, and d are covered for the second state model. Hydrogen demand (fuel input) is fixed as an input parameter as did Lahnaoui et al. (2018).

Table 4. 1: Definition of the various parameters in the second-state model

Parameter	Definition	Value	Explanation
a	Growth rate of conventional vehicles (ICEVs)	0.05	Based on literature (Leibling, 2008b) and validated in chapter 3.
b	Attack rate of HBVs on ICEVs	2.2e-9	Attack rate depends on the scenario i.e. for the extreme scenario the attack rate will be low
c	Hydrogen efficiency	3.11e-10	How many vehicles does the infrastructure support?
d	Growth rate of HBVs	0.05	The growth rate of HBVs is also set to 5% for all predators following the UK's vehicle growth rate over the last 50 years.
Conventional Fuel	Conventional Fuel consumed in a year	3.2e10 kg/year	The amount of conventional fuel consumed to support the private fleet of 3.2 million vehicles considering A4.7.
Hydrogen fuel	Total amount of hydrogen fuel consumed (kg/yr)	See table 4.2	The amount of hydrogen fuel consumed in a year depends on the demand.

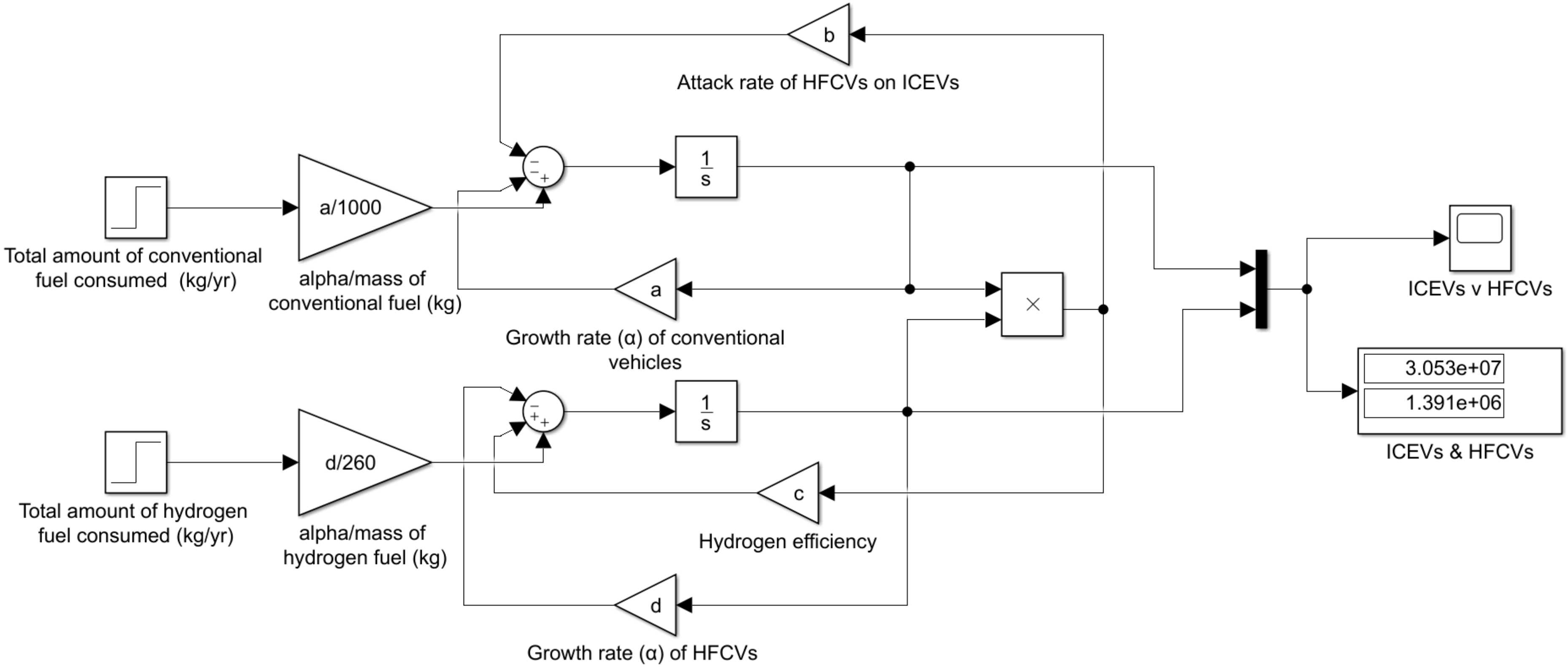


Figure 4. 1*: represents the simulation model considering ICEVS v HFCV*

4.2.6 Model Validation

The model was validated by determining the capacity of different HRSs and the number of HBVs that can be supported by the stations operating at maximum capacity/efficiency. This was then used to assess whether the model utilising predator-prey aspects was able to project reasonable results. This will form the basis to extend the model to represent more realistic scenarios.

4.2.6.1 Hydrogen Capacity

This section considers the hydrogen capacity for different types of stations based on the solar powered hydrogen station in Swindon (Crosse, 2014), and the other a large SMR station (Almansoori and Betancourt-Torcat, 2016a). From the literature review it is evident that renewable energy-based power stations are being invested in for short-term and larger SMR stations will play a huge role in meeting demand. This will allow both to be considered in terms of capability and practicality of meeting the UK's hydrogen demand.

Table 4. 2: Shows the capacities of different types of RS in kg/day and kg/year.

Station type	RS capacity kg/day	Capacity kg/year (100% efficiency)	Reference
Small	80	29120	(UKH2Mobility, 2013)
Small (hydrogen solar-powered electrolysis RS)	200/212	73000/77380	(UKH2Mobility, 2013; Crosse, 2014; Reddi et al., 2017; Tlili et al., 2020)
Medium	400/420	146000/153300	(UKH2Mobility, 2013; Tlili et al., 2020)
Large (SMR)	1000	365000	(UKH2Mobility, 2013; Almansoori and Betancourt-Torcat, 2016b; Reddi et al., 2017; Tlili et al., 2020)
Large	8064	2943360	(Mayer et al., 2019)

In the different scenarios, the impact of introducing HFCVs into the road transport market on ICEVs was assessed. The parameters selected are given in the table below:

Table 4. 3: Storage capacity parameters selected for the model for the HFCV and the range-extender (RE)

Vehicle type	Storage capacity (Kg)	Fuel Consumed (kg/year per vehicle)	Reference
HFCV	5	260	(Toyota, 2016; Crosse, 2014; GCC, 2014; Hyundai, n.d.)
HFC-RE	1.5	78	(H2moves Vehicles, n.d.)

As stated in A4.7 the HBVs will be refuelled once a week when calculating the amount of fuel consumed per year per vehicle. The hydrogen demand will initially be calculated using a 200 kg/day RS as the baseline (UKH2Mobility, 2013) and the number of HBVs supported by it to assess the model and select appropriate parameters. This allowed the data to be simulated assessing the level of hydrogen penetration expected in literature and whether the second order model projected the similar figures. In this case, the hydrogen capacity will be simulated at 100% (Rahmouni et al., 2016) to determine as the baseline to allow comparison with the results obtained from the literature. If the results correlated strongly, then the model is plausible, predicting the number of HBVs accurately. This will then allow different efficiencies to be modelled in terms of meeting the capacities of the HRS. This close correlation is only achieved with 100% efficiency (Mayer et al., 2019) (i.e. the hydrogen infrastructure is operating under maximum productivity) and under different efficiencies (more realistic scenarios) will represent different correlations.

4.3 Results

4.3.1 Modelling and testing the plausibility of the second order LVM

The growth of conventional vehicles is accurately represented by the growth model developed in Simulink indicating that the model developed does represent the UK's growth (section 3.2). The LVM was then extended to encompass the growth model to assess the impact of introducing HFCVs as a competitor to conventional vehicles. To test the plausibility of the model the hydrogen demand was generated as an input to the model.

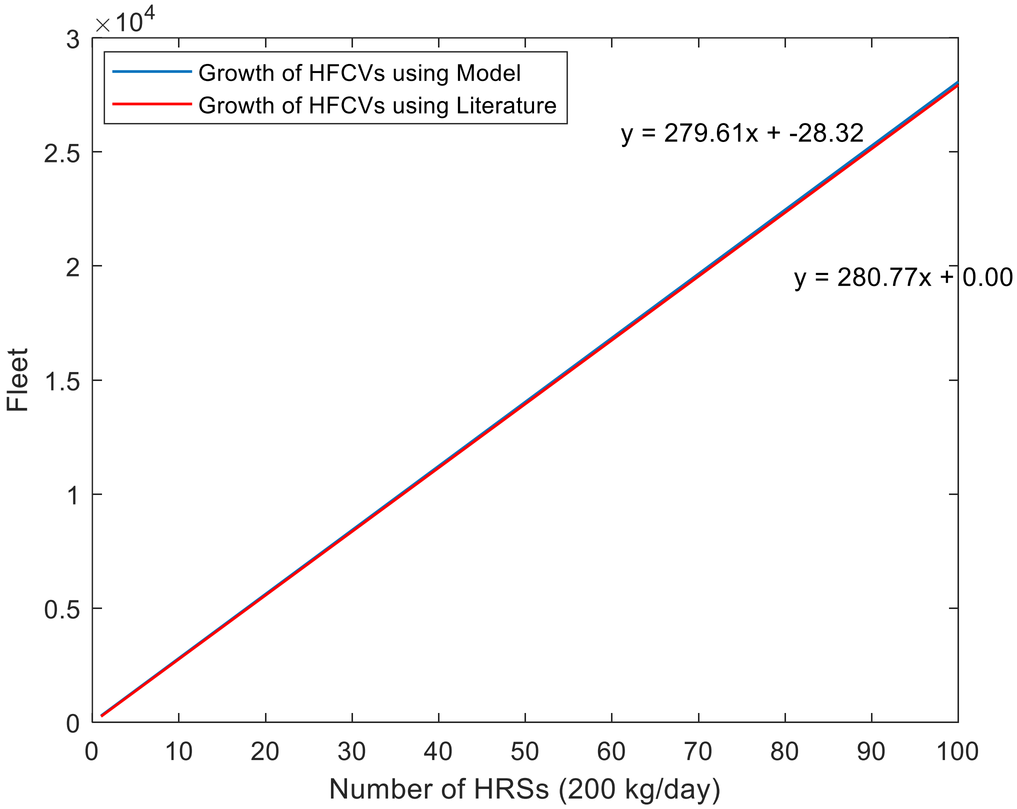


Figure 4. 2: Comparison between the growth of HFCVs between literature and the model considering 100 small RSs with a capacity of 200 kg/day

Figure 4.2 was generated using data from the literature depicting the relationship between the increase of HRSs with a capacity of 200 kg/day and the increase of HFCVs supported by it. Appropriate parameters (table 4.1) were selected ensuring that the model was set to operate at 100% efficiency and the results obtained from the simulations are depicted on the same graph. The number of vehicles supported by the network using the model are closely correlated with those obtained using literature with both supporting an R value of 1. The graphs demonstrate that the parameters selected for 100% efficiency are suitable and appropriate to simulate different scenarios as required.

4.3.2 Comparison of Hydrogen Refuelling stations for sustainable growth

The literature has presented a number of HRS/plants with varying capacities to produce and deliver hydrogen for near and long term solutions (UKH2Mobility, 2013; Almansoori and Shah, 2012). Currently, the emphasis is on building smaller 200 kg/day stations (Crosse, 2014). However, it may be cost effective in the long run to focus on larger stations with the capacity of 8064 kg/day or more with reduced output until demand increases. The following section provides an analysis on various stations mentioned in literature, their capacities and the number of vehicles that can be supported. Here HFCVs and HFC-REs are considered separately. The analysis also considers various strategies to promote and increase the number of HBVs in the road transport market.

4.3.2.1 The effect of station size

For the near to medium term, it is expected that small-sized stations will be built due to lack of demand and under-utilisation will be costly. However, building smaller sized stations will only extend the period of under-utilisation and investments in larger stations will reduce the period of under-utilisation. The advantage of near-term investment in small HRSs is that on-site reforming and electrolysis can be utilised with ease eliminating the need to transport the hydrogen and endure losses in terms in compression and liquefaction and thus the boil-off effect associated with liquid hydrogen (Elgowainy, 2014; Ratnakar et al., 2021).

From figure 4.3, the number of HFCVs supported by 100 HRSs at varying capacities (80 kg/day, 200 kg/day, 400 kg/day, 1000 kg/day and 8064 kg/day) are shown over a period of 40 years. In each case the number of vehicles supported by the network is negligible considering the entire private vehicle fleet. As shown in figure 4.4, conventional fleet consists of 31.8 million vehicles, and the network of 100 HRSs with the largest capacity of 8064kg/day each can only support 11,240 vehicles. The capacity of short-term smaller stations will have little impact on long-term planning and uptake of HFCVs because of the cost involved. It will be more effective to plan considering the endpoint with regards to the 2050 targets and considering the hydrogen network holistically.

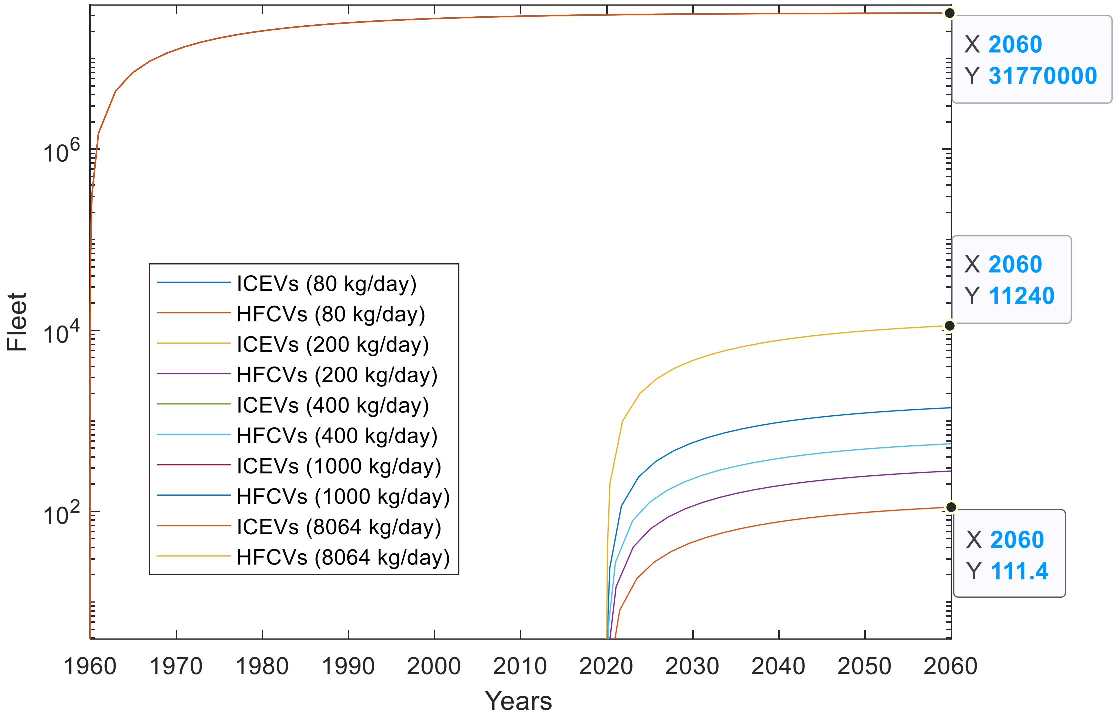


Figure 4. 3*: The graphs show the number of HFCVs supported by 100 HRSs with varying daily capacity of 80 kg/day, 200 kg, 400 kg/day, 1000 kg/day, and 8064 kg/day.*

From the literature, various roadmaps and plans by governmental bodies focus on instilling a pre-commercialisation network of stations. Some have proposed 100 HRSs for this period with small capacities ranging up to 200kg/day. From figure 4.4, it is clear that a network of 100 HRSs, with a daily capacity of 200 kg/day can only support 111.4 vehicles, assuming that they refuel at least once a week. A network of HRSs, with a daily capacity of 1000 kg/day, can only maintain a fleet of 1397 HFCVs, and a network of 100 HRSs with a daily capacity of 8064 kg/day, can only maintain a fleet of 11260 HFCVs.

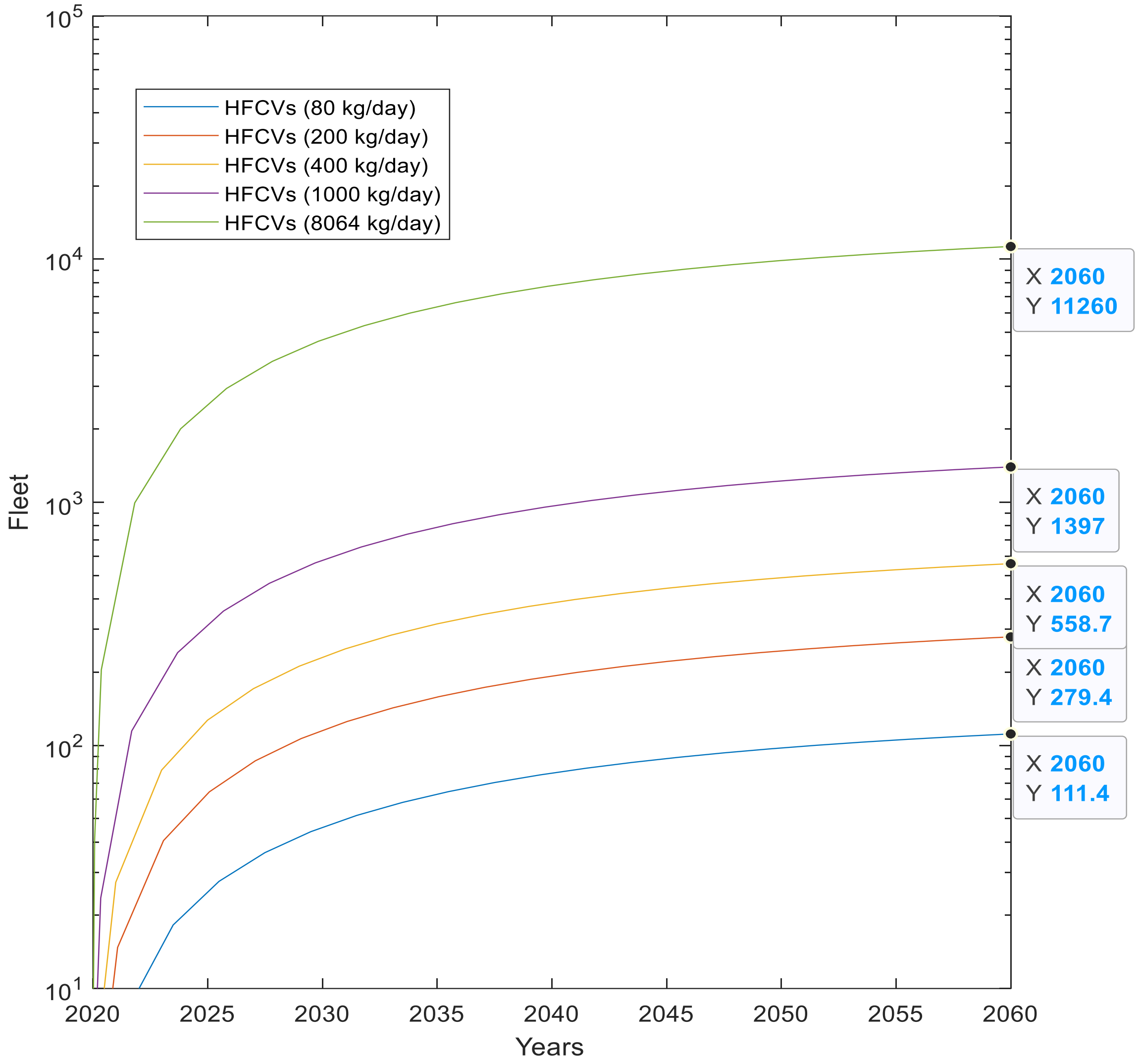


Figure 4. 4: A comparison of different networks of HRSs with varying capacities over a period of 40 years (2020-2060).

4.3.3 Hydrogen Fuel Cell Vehicles or Hydrogen Fuel Cell Range Extenders?

The graph below (4.5) represents the number of HFCVs, and HFC-REs supported by a network of small HRSs with a daily capacity of 200 kg/day. The same network of HRSs can support a number of 93,090 NFC-REs compared to 27,930 HFCVs. The percentage difference between investing in HFCVs and HFC-REs is 107.7%. The number of HFC-REs supported by the infrastructure is clearly greater, and with the electrical infrastructure already well-established is a promising option in introducing HBVs to the market for early adopters. Full hydrogen vehicles currently support a 5kg tank on average in the market. So fewer HFCVs are maintained compared to the 1.5kg hydrogen tank supported by HFC-REs.

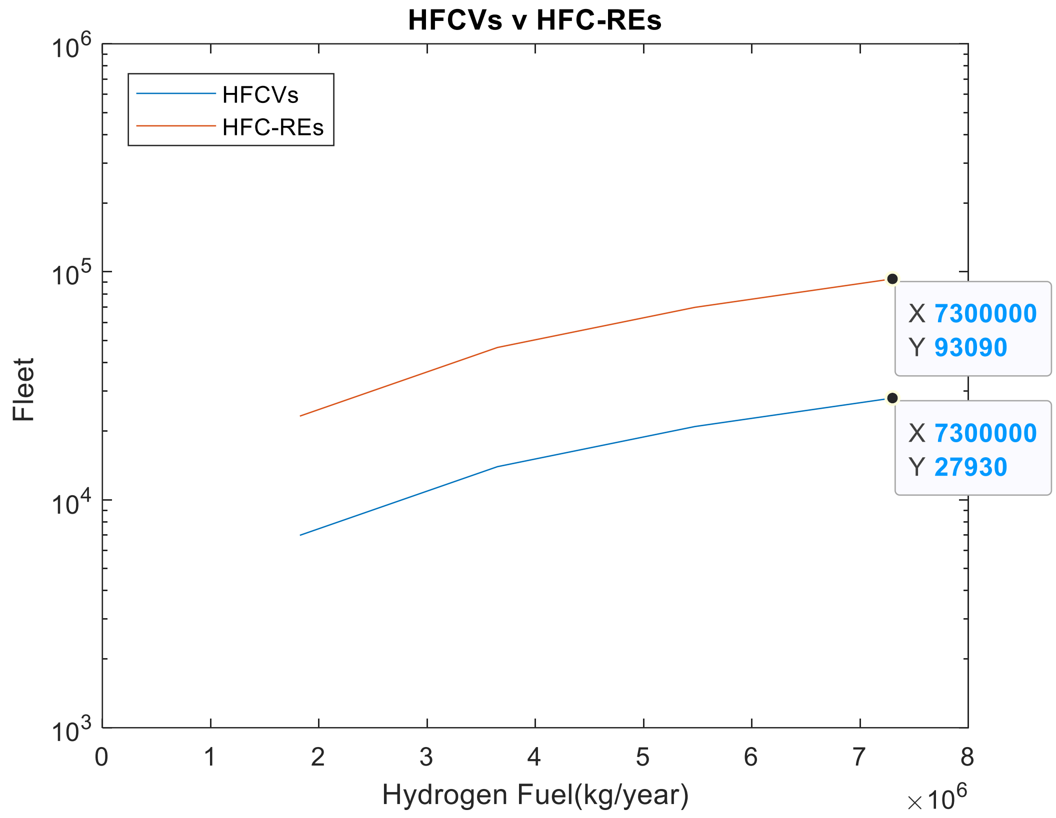


Figure 4. 5: Compares the number of HFCVs and HFC-REs supported by a network of HRSs with a daily capacity of 200 kg/day.

The results obtained from the second-order model demonstrate that the model is plausible with strong correlation with data calculated from the literature (figure 4.2). The results also indicate that larger stations are more beneficial in speeding up the transition to a hydrogen economy. Thus, shortening the period of under-utilisation of HRS. Furthermore, greater emphasis is required on HFC-REs to encompass the current electrical infrastructure and to allow more HBVs to be supported by the infrastructure available. A limitation in HFC-REs is that the primary source of energy will still primarily be conventional fuel and so still emitting emissions at the end use.

4.3.4 Current state of AFVs in the UK passenger vehicle market

Hybrid technology is the intermediate ground for the transition from fossil-based passenger vehicles to a renewable based one. Success of hybrids and EVs can potentially limit the investment in hydrogen. This section considers the scenario comparing the progress of hybrids and the impact on conventional vehicles thereof. The number of hybrids, plug-in hybrids, electric, range extenders, gas, vehicles using new technologies from UK's official statistics (DfT, 2018) were combined into one category as NFC-REs.

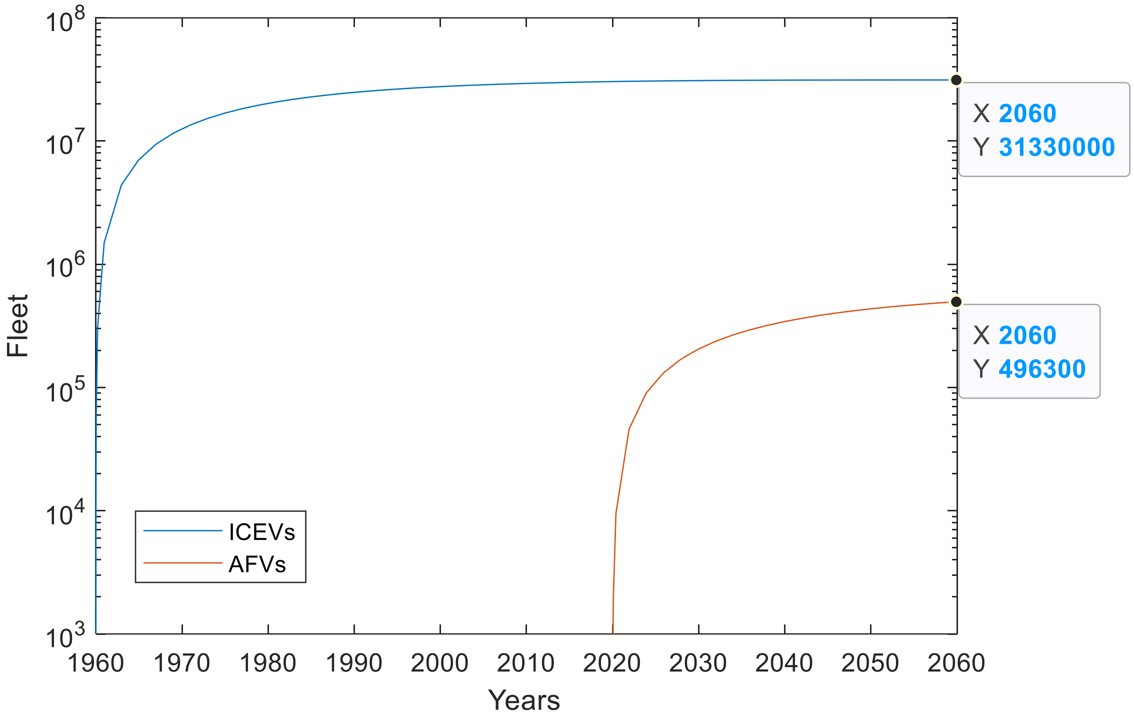


Figure 4. 6: Depicting the current number of AFVs in the market.

Figure 4.6 shows the number of AFVs registered in the UK by the end of 2018. The current level is depicted in comparison to conventional vehicles, where AFVs make up 1.58% of the fleet. Here, the number of NFC-REs is just under half a million in comparison to the approximately 32 million conventional vehicles on the road.

4.4 Discussion and Analysis

In response to the third research question, this chapter aimed to propose a dynamic model that considers the introduction of AFVs into the passenger vehicle market. It explored the model's plausibility to make accurate predictions in terms of the growth of HFCVs, and to consider their impact on conventional ICEVs. Different HRSs were considered to assess the most appropriate means of effective long-term sustainable planning for the sector.

The number of HFCVs supported by a network of 100 HRSs with a capacity of 200 kg/day were compared to the number projected by the model. This was intended to assess the plausibility of the second-order model. The relationship was expected to be positively linear, as depicted in figure 4.2. The R-squared value on the graph shows a perfect fit for the regression line as expected. Figure 4.2 shows the growth of HFCVs as the number of HRSs increases indicating a strong positive correlation with a R-squared value of 0.99. The percentage error between the two graphs is less than 0.01%. This level of accuracy was achieved by the selected parameters shown in section 4.2.5. Achieving a close correlation was significant to overcome the limitation of forecasting models. They do not have the relevant diffusion data to compare to especially when introducing new technologies (Park et al., 2011b). The close correlation will result in realistic projections proposed by scenarios.

For this research, it was assumed that investment in further construction will only occur as the demand for HFCVs increases after the initial period. The literature currently indicates that smaller RS will be built in the near future with low demand (UKH2Mobility, 2013). However, larger stations will have to be built sooner if the growth of HBVs is encouraged and reduce the under-utilisation period. Current interest by stakeholders and pre-commercialisation plans have focused on small HRS with 200 kg/day capacity. Stations with the capacity of 1000 kg/day are classified as large stations (UKH2Mobility, 2013). They will require hydrogen to be delivered to the site either by road or pipeline from a nearby facility adding to the cost (Reddi et al., 2017).

Figure 4.3 depicts scenarios of a 100 HRS being built of varying capacities ranging from 80 kg/day to 8064 kg/day. In the scenarios, it was assumed that the HRS will be operating at maximum capacity over the course of a year. This is unlikely to occur or maintain but essential in determining the effect of different stations sizes. In all the scenarios, even with 100 such stations, the number of vehicles supported is negligible when considering the entire passenger vehicle fleet and operating at maximum efficiency. There is no room for expansion to facilitate further growth in the sector. At 1000 kg/day, 100 HRSs could only support 139600 HFCVs, less than 0.5% of the conventional vehicle fleet.

The largest station considered from literature was the 8064 kg/day station (Mayer et al., 2019), which only supported less than 5% of the vehicles. When operating at maximum efficiency, the network of HRS could only support 1.12 million. Figure 4.4 depicts the hydrogen growth of different HRSs close-up, demonstrating that investing in HRSs < 1000 kg/day is not a practical solution in huge numbers. The number of conventional refuelling stations has seen a steady decline over the years. Over-investment in small scale HRS will encounter a significant number of stations to meet the demand in the medium to long term. Later investments in larger stations can result in the decline of smaller stations, which are being underutilised (Elgowainy, 2014).

One alternative is to focus on HFC-REs to increase the number of HBVs in the passenger vehicle fleet. A lower demand for hydrogen per vehicle (1.5 kg) means that each station can support more vehicles (figure 4.5). Utilising HFC-REs over HFCVs demonstrates that the percentage change in vehicles supported by the network of HRSs increases by 233.3%. However, there must be enough electrical infrastructure to supplement the growth requiring further investments in the electrical infrastructure to support the growth of NFC-REs. For hydrogen to become a prominent transport fuel, then investment in larger centralised plants must be considered sooner rather than later. At under-utilisation, there is a tendency of boil-off losses (below 25%) (Mayer et al., 2019) and can be avoided by siphoning excess hydrogen produced to other sectors and utilised as backup power to the grid when required. Hydrogen itself is a form of energy storage and can help meet energy demand in other sectors allowing stations to work at higher efficiencies from the start. This will benefit all industries involved, especially in reducing non-renewable electricity from the grid. HRS should also be used to home some electrical recharging points reducing the need for separate stations or journeys that drivers must undertake who purchase HFC-RE with dual-fuelling at the same time.

Hybrids and EVs are serious competitor with HBVs in determining whether HBVs will seek a percentage of the passenger vehicle fleet in the future or simply a portion of the range-extender market. Figure 4.6 shows that the number of other AFVs is just under half a million in the UK, so substantial work is required before becoming a dominant vehicle type. For HFCVs to enjoy 0.5% of the market, a substantial number of HRSs are required at current choice of station size. Only 139600 HFCVs can be supported if 100 1000 kg/day stations are opened that operate at maximum capacity continuously. For sustainable growth, larger stations are required that operate efficiently with the potential of expansion as the demand grows.

4.5 Conclusions and chapter summary

The purpose of chapter 4 was to evaluate the proposed model against current supply chain proposals demonstrating the ease of use and plausibility. The modified LVM was able to represent the growth of conventional and HBVs through the integrated growth model.

Depending on the strategy selected, introducing HBVs, or other AFVs will displace conventional vehicles. However, with a more robust strategy a much greater infrastructure is required, especially for HBVs. Short-term HFC-REs can play an important role, however range extender vehicles still consume a large proportion of fossil fuel. Introducing hydrogen through large, centralised plants is more economical in the near term. Despite not having a high demand, a hydrogen infrastructure should be pursued to shape the future of transport in the UK rather than simply reacting to social and political indicators as current models as is the current strains due to COVID-19 and the political pressures. This will also reduce the overall carbon targets for both the transport sector and other sectors.

The private vehicle sector comprises of different vehicle types and not just conventional and hydrogen-based vehicle. The second order model will be extended in chapter 6 to encompass other vehicle overcoming this limitation. This will also allow the role of hydrogen and other fuels to be envisaged and portray the best scenario for the UK, enabling stakeholders to take appropriate measures to make this projected future a reality. The alternative option is to look at similar technology introduced and its impact, such as non-FC hybrids. The next chapter considers the second order model in a case study, rigorously testing it against other proposals.

The results of the second-order model are summarised below:

1) The growth of HFCVs simulated from the model correlated to that obtained from the literature. By adjusting the parameters, the model can predict the growth accurately with an error of less than 0.01%.
2) Current definitions of large HRSs need to be changed to accommodate larger capacities, because 100 HRSs of 8064 kg/day capacity each can only provide hydrogen for 11,360 vehicles.
3) HFC-REs must be utilised to bridge the gap between pre-commercialisation and an established market.
4) The utilisation of HFC-REs over HFCVs increases the capacity of the network to support an increase of 233.3% vehicles.
5) Large centralise stations must be developed as soon as possible for sustainable growth in the sector regardless of the hydrogen demand for vehicles.

Chapter 5: Case Study (UK) and scenario development

5.1 Introduction

In this chapter, the second order LVM was applied to the UK to critically evaluate the model against current supply chain (SC) proposals and frameworks in accordance with objective 4. The model's capabilities are illustrated through the application of a case study using current proposals for the UK as the backdrop. Some of the scenarios developed in the literature are unrealistic, so therefore the analysis of the UK eliminates some of these unrealistic scenarios considering current policies and progress by the UK. This will also provide feedback to propose realistic scenarios informing policies in decarbonising the private fleet using different technologies.

The chapter is split into three broad sections considering the proposals selected from literature, results, and discussion. The first section considers proposals/scenarios selected from the literature using the UK as a backdrop. These are used to determine a standard timeframe to simulate the data/scenarios for consistency. This is followed by the formation of penetration scenarios for hydrogen. Next, the results section outlines the various hydrogen demand over the periods of 2020-2060, followed by the results simulated for different scenarios and then the hydrogen 'space'. Finally, the discussion section is followed by the chapter summary and the lessons learned.

5.2 Determining a standard timeframe from current proposals

As discussed in the literature review, three proposals were selected to engage current projections for hydrogen demand. These proposals were selected because they provide a comprehensive data and scenario for the UK covering a breadth of time-period they covered. To analyse the scenarios using the modified second-order LVM, then the data available must also be complete. The UKH2Mobility report outlined the UK's proposal build a pre-commercialisation infrastructure for HBVs (UKH2Mobility, 2013, 2016, 2020). The outlook forecasted by the UKH2Mobility group has been used as the extreme case scenario where limited infrastructure is developed keeping the role of hydrogen's role in the private vehicle at minimum. Scenarios developed by Almansoori and Shah were considered as the second-moderate scenario because their work has been used extensively in modelling hydrogen for private vehicle fleet in the UK with complete data (Almansoori and Shah, 2012). There are a limited number of studies considering the UK as a backdrop, thus data is often incomplete especially with variations in research objectives and modelling approaches. The third scenario selected from literature stems from the work of Moreno-Benito et al (2017) forming the third, best-case scenario.

Table 5. 1: Some approaches used to predict the hydrogen demand for the UK.

Model Type	Year Period	Year	Ref
Multi-period stochastic model	2005 - 2030	2012	(Almansoori and Shah, 2012)
Logistic Diffusion Model	2020-2070	2017	(Moreno-Benito et al., 2017)
GIS MARKAL	-	2009	(Strachan et al., 2009)
UKH2Mobility Report	2015-2030	2013	(UKH2Mobility, 2013)
Mixed methods approach	2015-2030	2016	(Southall and Khare, 2016)
UK MARKAL	- 2050	2013	(Balta-Ozkan and Baldwin, 2013)

Determining the hydrogen demand is a dynamic process that encompasses several factors that are open to interpretation by the researcher. One of the key issues surrounding the determination of hydrogen demand is the saturation point of HFCVs using UK as the backdrop. This can be seen from table 5.1 where six studies conducted between 2009 to 2017 have considered different year period for HFCVs to penetrate from 2005 to 2070. The purpose here was to assess the timeframe in which hydrogen is expected to become a dominant transportation fuel. Although on average, it is expected that 50% of the UK's road vehicle will be switched to hydrogen by 2050. However, some studies have predicted this to happen sooner with the hydrogen demand projections (Almansoori and Shah, 2012), while others later (Moreno-Benito et al., 2017). To gauge the effectiveness of the proposals, the data from the three proposals are simulated across the average time, which is 2020-2060 to provide a constant measure for all the models.

The purpose of utilising the data from the three sources was, first to test the second-order model developed more rigorously to see if the model utilising predator-prey aspects could project reasonable results. Secondly, to ascertain whether the current proposals are realistic or over/under predicting the use of hydrogen as a transportation fuel. Third, three of the most prominent studies forecasting the penetration and growth of HBVs for the UK were covered with complete data. In conjunction with the latest UK emissions targets and policies, the outcome of this chapter will help develop more realistic scenarios to decarbonise the UK's passenger vehicle fleet by 2050.

5.3 Formulating penetration scenarios for hydrogen

Researchers have largely based the hydrogen demand on scenarios developed; the number of scenarios are chosen by the researchers and vary in number, for instance six scenarios were selected by Liu et al (2012), whereas Tlili et al (2020) chose three scenarios. A large number of studies have limited the scenarios to three, depicting the "worst", "middle" and "best" paths for HFCVs to penetrate the private vehicle market (Almansoori and Shah, 2012; Talebian et al., 2019a; Tlili et al., 2020). As a result, a three-case scenario is proposed for this case study of extreme-case, moderate-case, and best-case scenarios. These are outlined as follows:

Extreme case scenario: This is based on the number of HRS remaining as they are until 2060. Further HRS built will assume capacities up to 1000 kg/day, but due to alternative vehicles such as hybrids and EVs, the benefits of hydrogen are outplayed by the cost and effort of installing an effective infrastructure without a sustainable demand. Many studies have assumed scenarios of minimal penetration of HFCVs into the market; both in terms of the worst-case scenario (Talebian et al., 2019a; Seo et al., 2020) and the best-case scenario (De-León Almaraz et al., 2015b; Lahnaoui et al., 2019).

Moderate case scenario: Here, it is assumed that half of the conventional vehicles will be replaced by HBVs by 2060 regardless of whether they are HFCVs or HFC-REs. In addition to on-site stations, off-site stations are also utilised with a centralised network. This is based on the work of Seo et al., (Seo et al., 2020) who proposed that once HFCVs attain a 20% share of the market, the strategy was switched from decentralised to centralised storage system.

Best case scenario: Some studies have considered a scenarios where HFCVs attain a 100% market share (Agnolucci et al., 2013; Rahmouni et al., 2016). However, in this case the best-case scenarios will assume 90% market share with the remaining utilising alternative fuels by 2060. Extensive hydrogen and electrical infrastructure are in place, with renewable energy utilised to meet a quarter of the energy consumed.

In all three cases, the hydrogen demand is determined for the year 2060. Currently, proposals are made to stop manufacturing conventional vehicles and reduce fossil fuel consumption by 80% by 2040 (DfT, 2009a; HM Government, 2018). Alongside these objectives by the government, most forecast models have used a similar timeline. In effect, the UK can take one of three routes and start planning from now to realise that route by 2060. These three case scenarios can be used as a benchmark to realise the role hydrogen is yet to play in the transportation sector. Table 5.2 below depicts the parameters used in the modelling for all three scenarios.

Table 5. 2: Parameters for the second-order model (ICEVs v HFCVs) simulation.

Parameter	Definition	Extreme	Moderate	Best case
a	Growth rate of conventional vehicles (ICEVs)	0.05	0.05	0.05
b	Attack rate of HBVs on ICEVs	2.1e-9	4e-9	8e-9
c	Hydrogen efficiency	9.74e-11	9.74e-11	9.74e-11
d	Growth rate of HBVs	0.05	0.05	0.05

Currently, 15 HRS operating in the UK, with 5 planned more stations planned (Netinform, a2019). If each station has an upper capacity of 200kg/day of hydrogen, then it is sensible to assume that by 2020 the UK will produce 1.46×10^6kg/year of hydrogen solely for road vehicles. For the extreme-case scenario, it is assumed that the progress made will stagnate and remain as it is. For the moderate-case scenario, it is assumed that half of the conventional vehicles will be replaced by HBVs. So, therefore, 15 million vehicles on the road in 2060 will be displaced by HBVs. The hydrogen required will primarily depend on whether the vehicles are HFCVs, HFC-REs or an equal number of both. The best-case scenario assumes that 90% of the vehicles on the road will be HBV. As a result, the hydrogen required to meet the refuelling demand of 27 million vehicles can be calculated accordingly.

For the transition to a hydrogen economy to occur, most vehicles on the road must be hydrogen-based regardless of whether they are HFCVs or HFC-REs. To envisage the transition's magnitude, it can be argued that a total displacement of the approximately 30 million conventional vehicles by HBVs is necessary. This allows us to calculate the total demand of hydrogen if this scenario is accepted, as shown in table 5.8. The demand for hydrogen is calculated separately for both HFCVs and HFC-REs. The amount of hydrogen demand includes the possibility of fluctuations, in that some drivers may refuel their vehicle more than once a week, e.g. taxi driver or those who must travel to work etc.

5.4 Results

Considering the UK's policies and emission targets represented in sections 3.2.2 and 4.2.2, the optimal design for the UK is to consider the implementation of a future hydrogen infrastructure by 2050 to meet these targets. The base-case used in this instance was the study carried out by Almansoori and Shah (Almansoori and Shah, 2012) because it is a well-established study for the UK and the corresponding hydrogen demand data is available. This presented the upper limit of the hydrogen demand in that the entire fleet will consists of either HFCVs or HFC-REs. The following section considers the hydrogen demand over this period.

5.4.1 Assessing the hydrogen demand over the period 2020-2060

The timescale often selected by researchers for hydrogen to penetrate falls between the years of 2005-2070 as indicated in table 5.1. Some of the projections are optimistic (Almansoori and Shah, 2012), while others are too cautious (Moreno-Benito et al., 2017). All projections were simulated and presented in the results assuming that the HRS operate at 90% of their capacity. This is because it is highly unlikely that continual investment in HRS will be made if the demand for hydrogen is not there; therefore, demand and HRS are expected to grow together.

Table 5.3 shows the scenarios modelled in the second-order model by using the data from the study of Almansoori and Shah (2012). Figure 5.1 below demonstrates the difference between HFCVs and HFC-REs in best case scenario of 70%; 11.8 million HFCVs can be supported in contrast to 38.8 million HFC-REs.

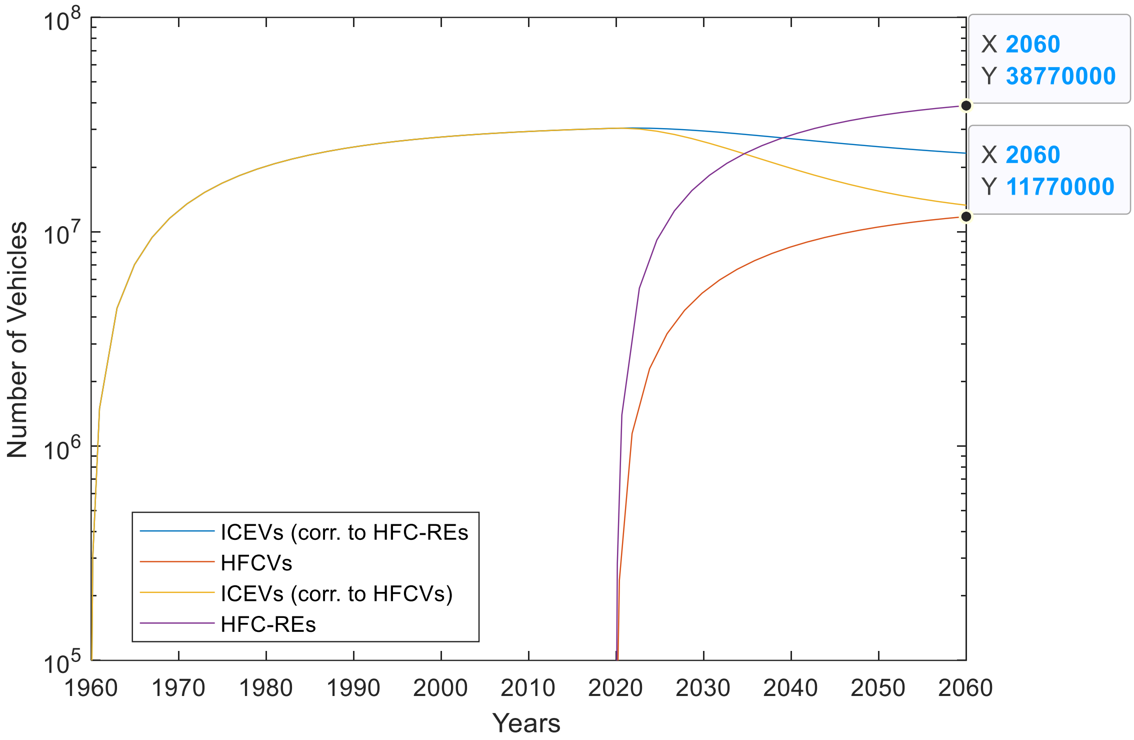


Figure 5. 1: The best-case scenario simulated using data from Almansoori and Shah using both HFCVs and HFC-REs.

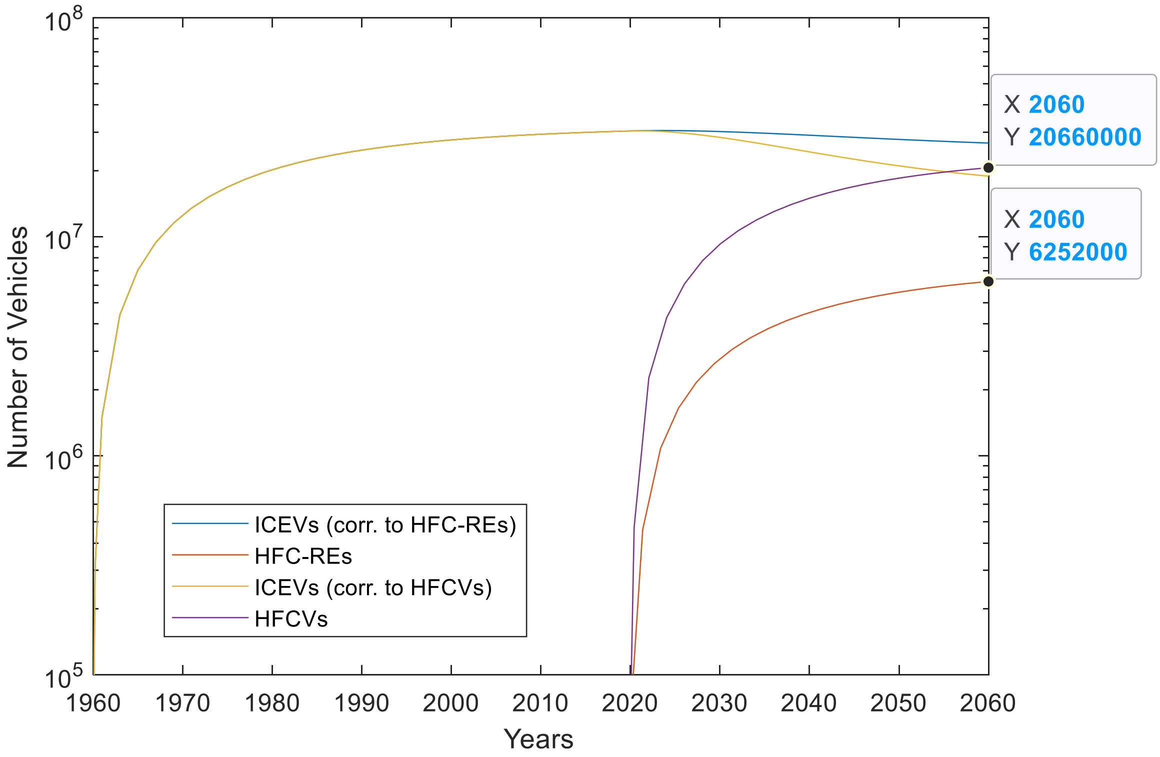


Figure 5. 2: Best case scenarios simulated from the data sourced from Moreno-Benito et al showing both HFCVs and HFC-REs

Moreno-Benito et al (Moreno-Benito et al., 2017) suggested in their work that the hydrogen transition can attain 50% of the market share by 2070 and full coverage by 2120. The data were simulated across 2020-2060 rather than the 5-year intervals from 2025-2070 (see table 5.4). This was done to provide consistency across all the different projections made in the literature. Again, both HFCVs and HFC-REs were simulated separately and figure 5.2 demonstrates the best-case scenarios consisting of 6.25 million HFCVs or 20.7 million HFC-REs.

Table 5.5 represents the data from the UKH2Mobility report simulated in the model assessing the impact of introducing hydrogen into the vehicle sector. Figure 5.3 depicts the best-case scenario extracted from the UKH2Mobility report. It shows that introducing hydrogen for HFCVs has a negligible impact on conventional vehicles when simulated to 2060 from 2020.

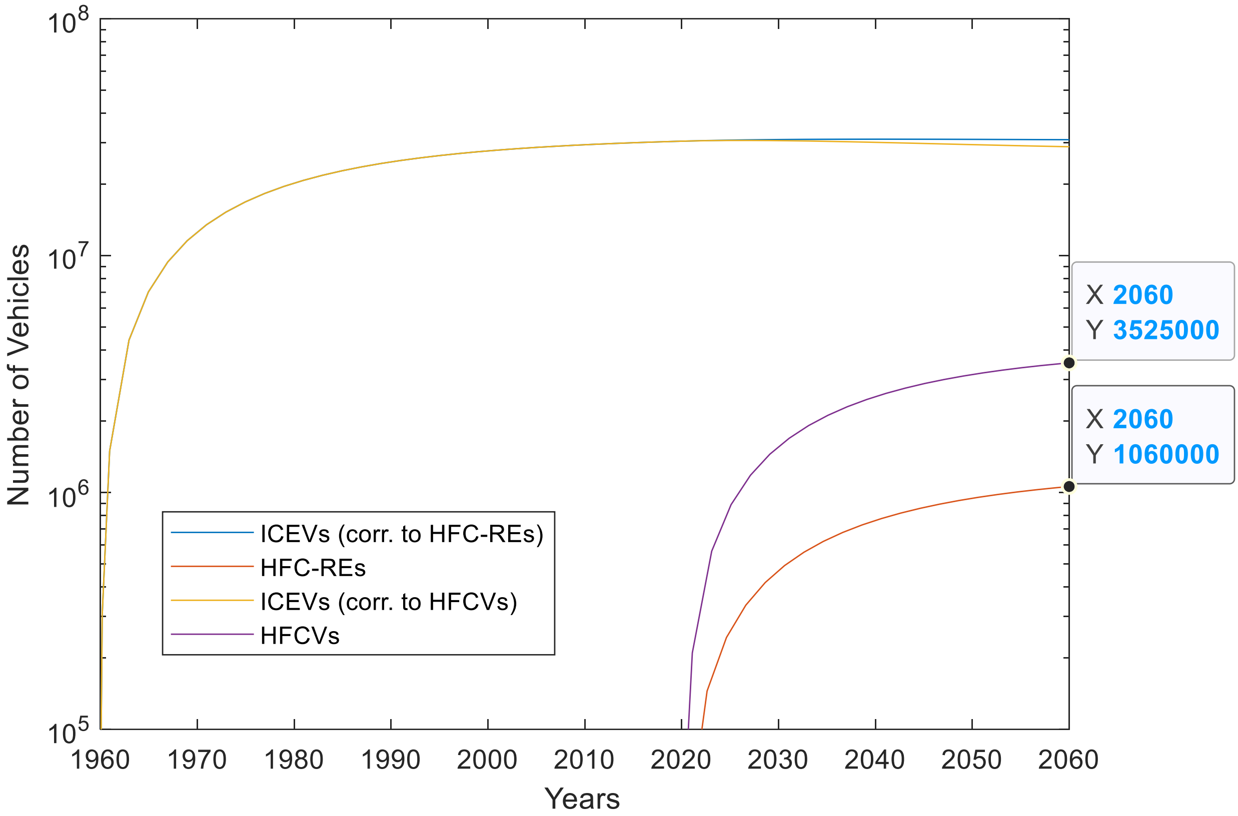


Figure 5. 3: The best-case scenario from the UKH2 Mobility report for both HFCVs and HFC-REs

Table 5. 3: Hydrogen demand calculated by Almansoori and Shah (Almansoori and Shah, 2012) simulated in the dynamic model.

Time Period, t(yr)	Scenario k, (%)	Demand, D (t/d)	Demand kg/day	Demand kg/d (x^6)	Demand kg/yr	HFCVs	HFCVs 90%	HFC-REs	HFC-REs 90%
2020-2060	5	670	670000	0.67	2.45E+08	9.41E+05	8.47E+05	3.14E+06	2.82E+06
	15	2009	2009000	2.009	7.33E+08	2.82E+06	2.53E+06	9.40E+06	8.41E+06
	20	2679	2679000	2.679	9.78E+08	3.76E+06	3.37E+06	1.25E+07	1.12E+07
	25	3349	3349000	3.349	1.22E+09	4.70E+06	4.20E+06	1.57E+07	1.40E+07
	30	4018	4018000	4.018	1.47E+09	5.64E+06	5.05E+06	1.88E+07	1.67E+07
	40	5358	5358000	5.358	1.96E+09	7.52E+06	6.73E+06	2.51E+07	2.22E+07
	50	6697	6697000	6.697	2.44E+09	9.40E+06	8.36E+06	3.13E+07	2.75E+07
	60	8037	8037000	8.037	2.93E+09	1.13E+07	1.00E+07	3.76E+07	3.30E+07
	70	9376	9376000	9.376	3.42E+09	1.32E+07	1.17E+07	4.39E+07	3.85E+07

Table 5. 4: Fleet simulated using data from Moreno-Benito et al (Moreno-Benito et al., 2017).

Year	Hydrogen demand kg/day	Hydrogen demand kg/year	HFCVs (Literature)	HFCVs (Lit) 90%	HFCVs (Simulink) 90%	HFC-REs (Literature)	HFC-REs (Lit) 90%	HFC-REs (Simulink) 90%
2020 - 2060	68569	25027685	96260.327	86634.3	8.66E+04	320867.76	288781	2.89E+05
	137131	50052815	192510.83	173260	1.73E+05	641702.76	577532.5	5.77E+05
	247804	90448460	347878.69	313091	3.13E+05	1159595.6	1043636	1.04E+06
	411152	1.5E+08	577194.15	519475	5.19E+05	1923980.5	1731582	1.73E+06
	674657	2.46E+08	947114.63	852403	8.52E+05	3157048.8	2841344	2.83E+06
	1054193	3.85E+08	1479924.8	1331932	1.33E+06	4933082.6	4439774	4.41E+06
	1706906	6.23E+08	2396233.4	2156610	2.15E+06	7987444.7	7188700	7.12E+06
	2575720	9.4E+08	3615914.6	3254323	3.25E+06	12053049	10847744	1.07E+07
	3687994	1.35E+09	5177376.2	4659639	4.64E+06	17257921	15532129	1.53E+07
	4956109	1.81E+09	6957614.6	6261853	6.23E+06	23192049	20872844	2.05E+07

Table 5. 5: The hydrogen demand projected by the UKH2Mobility report – the number of small, medium and large stations are an approximation.

H2Mobility report		Small	Medium	Large	Total	Capacity kg/day	Capacity kg/year	HFCV	HFCVs	HFC-RE	HFC-REs
Capacity (kg/day)		80	400	1000					**90%**		**90%**
2015-2020	2020-2060	65			65	5200	1898000	7300	6570	24333.33	1.19E+04
2020-2025			330		330	132000	48180000	185307.69	1.67E+05	617692.3	5.56E+05
2020-2030			750	400	1150	700000	255500000	982692.31	8.83E+05	3275641	2.94E+06
Total							305578000	1175300	1.06E+06	3917667	3.50E+06

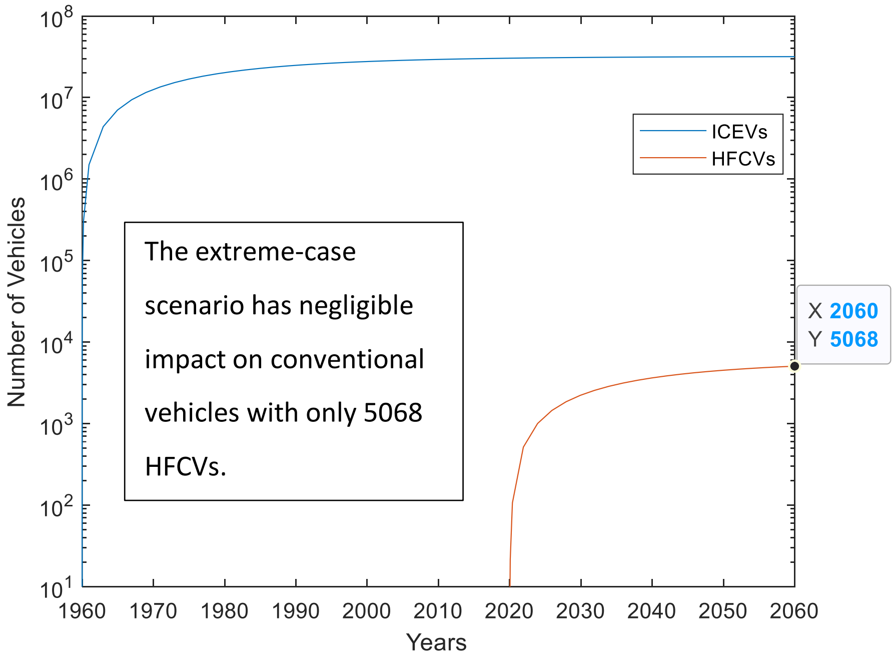
5.3.2 Results simulated for different scenarios

In the previous section, different scenarios from the literature were simulated to analyse the hydrogen forecasts for the UK. In this section, three scenarios are developed to investigate the impact on the private vehicle market to eliminate unrealistic scenarios. The second-order modified LVM is used simulate these scenarios. Table 5.6 outlines the three scenarios of extreme, moderate, and best-case scenarios. Since the growth for conventional vehicles has been approximately 5% for the last 50 years, it is more likely that the vehicle type replacing ICEVs will be manufactured and sold at a similar growth as mentioned by Agnolucci et al. (2013). The results from the simulations encompassing the above parameters are shown below for ICEVs v HFCVs. The fuel input selected for the extreme scenario for the introduction of HFCVs is based on having 20 RS with a capacity of 200 kg/day (see table 5.6). 20 RS will be able to support 5068 HFCVs.

Table 5. 6: Table representing the simulated scenarios based on a 200 kg/day RS by 2060.

Scenarios	**Conventional fuel input kg/yr.**	**ICEVs**	**Hydrogen fuel input kg/yr.**	**HFCVs**	**Year**
Extreme	3.2e10	3.17e6	1.46e6	5068	2060
Moderate	3.2e10	5.046e7	5e9	17.2e6	
Best case	3.2e10	1.539e7	9e9	30.7e6	

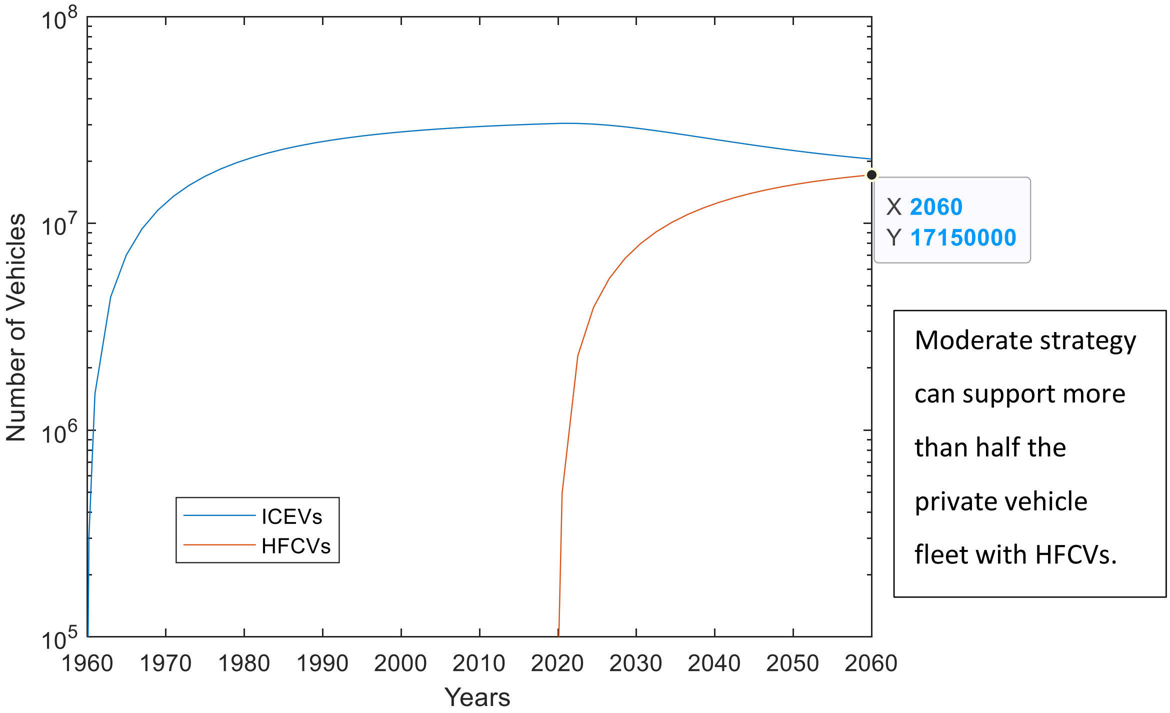
The moderate-case scenario assumes that HFCVs will capture 50% of the fleet, whereas the best-case scenario assumes that 90% of the fleet will be HFCVs by 2060. In addition to that, the hydrogen infrastructure is assumed to be operated at 90% of its capacity. Initially, it is expected that HRS will be under-utilised before operating at higher efficiencies. In the long-term, HRS are expected to operate near maximum capacity. It is highly likely, that with alternative fuel, as with electricity, smart systems synchronising RS and vehicles will inform drivers of nearest stations and their availability. If a RS does dispense all its fuel in a day, its reserve can also be utilised from storage, increasing capacity, thus reducing fuel shortage.



The extreme-case scenario has negligible impact on conventional vehicles with only 5068 HFCVs.

Figure 5. 4: Extreme scenario of hydrogen's introduction (business as usual)

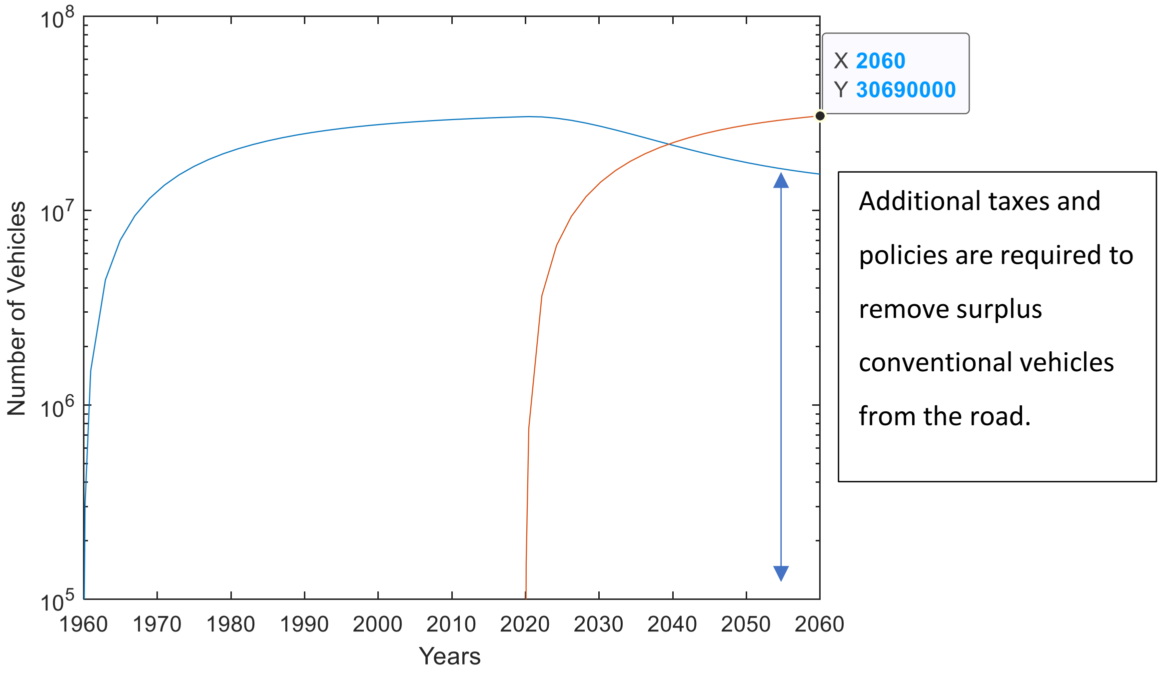
Figure 5.4 shows the simulation graph obtained for the extreme scenario of introducing hydrogen. This has minimal impact on the number of conventional vehicles suggesting that hydrogen will not penetrate the road vehicle market at less than 0.5%.



Moderate strategy can support more than half the private vehicle fleet with HFCVs.

Figure 5. 5: Moderate scenario of hydrogen's introduction.

The moderate scenario obtained from the simulations is depicted in figure 5.5, showing that hydrogen will obtain a sizeable share in the market of 57.2%. However, conventional vehicles will have to be removed from the sector at the end of their lifetime. Figure 5.6 below represents the best-case scenario for hydrogen to compete against conventional vehicles.



Additional taxes and policies are required to remove surplus conventional vehicles from the road.

Figure 5. 6: Depicts the best-case scenario of hydrogen's introduction into the vehicle market replacing conventional vehicles.

Here, the amount of conventional fuel for all three scenarios was maintained at 3.2e10 kg/yr. In this case, reduction in fuel is not causing ICEVs to reduce in number, but rather the introduction of HFCVs. As the number of HBVs increases, the number of conventional vehicles is reduced based on the attack rate. This is expected in the absence of a predator, the prey or established technology will continue to flourish until fuel supplies diminish. For the best-case scenario, HBVs will have enough vehicles to displace conventional vehicle fleet. To drive the conventional vehicles down making drivers switch to HBVs, additional taxes on fuel and limited supply will need to be enacted.

5.3.3 Hydrogen Space

To oversee the transition of the UK's road transportation to hydrogen from a fossil-fuel based, it is essential to develop a sense of the 'space' available. Table 5.7 shows the hydrogen demand calculated according to the three scenarios outlined in section 5.3.2. The hydrogen demand calculated is based on the number of UK's passenger vehicles only (excluding vans and other types of vehicles). The number of road vehicles projected for 2020 in the UK is approximately 30 million, and this figure will be used as the benchmark to define the 'hydrogen space'. If all vehicles are to be replaced by HBVs, then the hydrogen space to be filled consists of 30 million vehicles + 5% growth. However, since EVs and other alternative fuel vehicles (AFVs) will also play a role in the future for road transportation, the 5% growth expected in the subsequent years is not included in the 'hydrogen space'. Since HBVs consist of both full HFCVs and range extenders, it is crucial to define the proportion of each to make more accurate projections for the required hydrogen to meet the demand.

Table 5. 7: The hydrogen demand calculated for the three scenarios by 2060 with HRS operating at maximum capacity.

Scenarios	Percentage of HBVs used to estimate demand	Hydrogen demand by 2060 (x10^9 kg/yr)	Number of HFCVs supported (x10^3)	Number of HFC-REs supported (x10^3)	Number of HBVs (50:50) supported (x10^3)
Extreme Case		1.46	5,615	18,718	8,639
Moderate Case	100% HFCVs	3.9	15,000	50,000	23,076.9
	100% HFC-REs	1.170	4,500	15,000	6,923.1
	50% each	2.535	9,750	32,500	15,000
Best Case	100% HFCVs	7.8	30,000	100,000	461538.5
	100% HFC-REs	2.34	9,000	30,000	13,846.2
	50% each	5.07	19,500	65,000	30,000

Table 5.8 demonstrates the difference between full HFCV and using hydrogen as a RE. Investing in HFC-REs requires significantly less investment in infrastructure as only 2500 million kg of hydrogen is required as compared to the 8000 million kg required for HFCVs. This is a more promising option in a HEV, replacing the ICE with a FC system to increase the range.

Table 5. 8: Number of HFCVs and HFC-REs maintained by the infrastructure by 2060 (Best case scenario to achieve decarbonisation).

ICEVs	HFCVs	Hydrogen consumed (kg)	ICEVs	HFC-REs	Hydrogen consumed (kg)
6.03e6	27.32e6	8e9	5.5e6	28.44e6	2.50e9

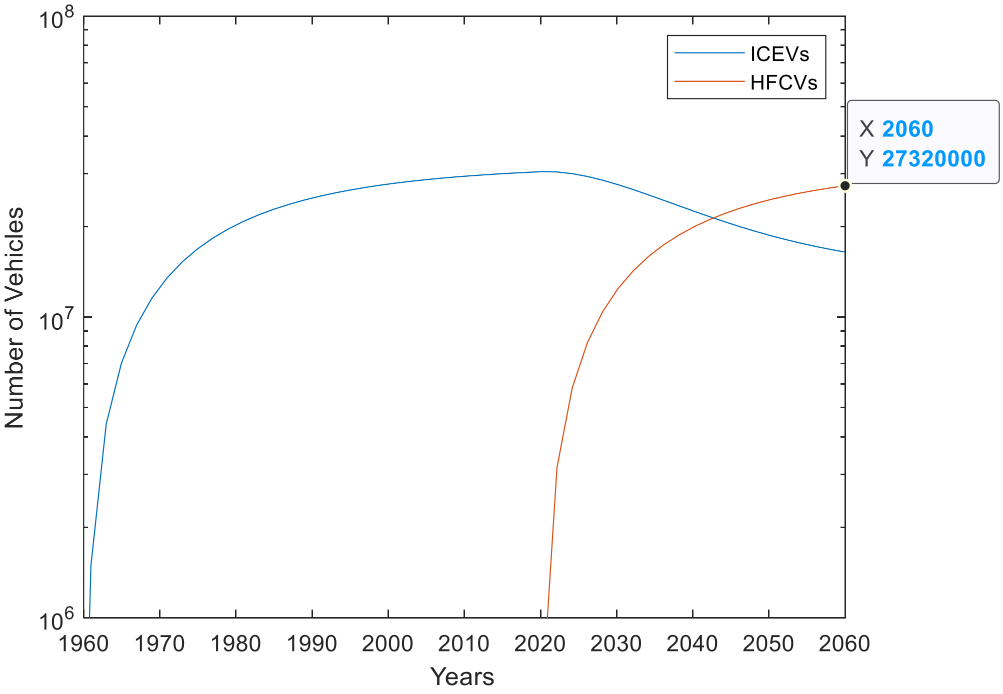


Figure 5. 7: Best-case scenario to replace the ICEVs from the current passenger vehicle fleet with HFCVs

Figure 5.7 represents the best-case scenario for HFCVs utilising $8\times 10^9 \text{kg}/H_2$, whereas figure 5.10 shows the best-case scenario for HFC-REs utilising only $2.5 \times 10^9 \text{kg}/H_2$.

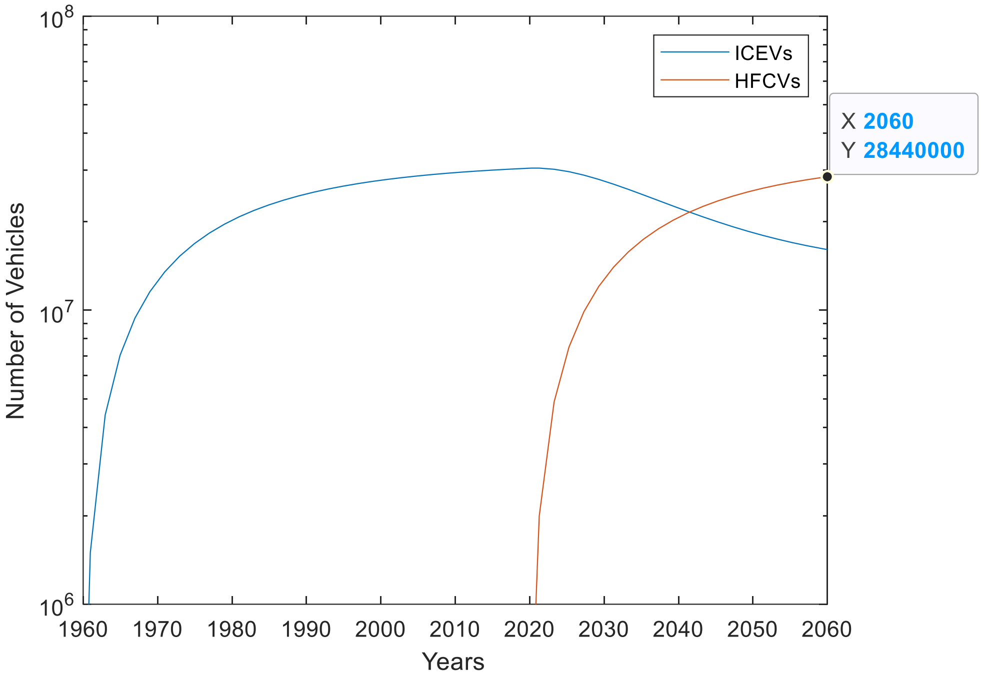


Figure 5. 8: Best-case scenario to replace conventional vehicles with HFC-REs

Current projections of hydrogen demand and infrastructure growth need to be revised if hydrogen is to play a significant role in providing tomorrow's transportation needs. Hydrogen can play a key role in the future of road transport to make the energy system more efficient.

5.4 Discussion and Analysis

5.4.1 Assessing the hydrogen demand over the period of 2020-2050

Forecasting the growth of hydrogen demand over the same period is a key factor in determining sensible and viable scenarios. Current scenarios from the literature, forecasting the growth of the UK's HFCV fleet were analysed using the modified second-order LVM over a constant period of 2020 – 2050.

Three scenarios were selected from UK based studies depicting the best-case (Almansoori and Shah, 2012), moderate-case (Moreno-Benito et al., 2017) and worst-case (UKH2Mobility, 2013) forecasts for the market penetration of HFCVs. Tables 5.3, 5.4, and 5.5 represent the data from the studies and the corresponding results from the modified second-order LVM.

For the best-case scenario, Almansoori and Shah (2012) determined a hydrogen demand of 3.42e9kg. According to their work, this demand was sufficient for hydrogen to capture 70% of the market share where the infrastructure became more decentralised, focusing on different geographical areas. This suggests that initially as demand starts to increase a more centralised infrastructure is favoured especially to meet the demand in hydrogen as proposed by Seo et al. (2020). However, as the market share of hydrogen continues to increase, multiple of centralised locations are required to meet the demand. So, naturally the infrastructure becomes more decentralised. The capacity of hydrogen on-board storage on average is 5kg (Toyota, 2016; Mirai, 2020), based on this the modified LVM has determined that only 11.7 million HFCVs can be supported by the infrastructure assuming the infrastructure operates at 90% of its capacity 24/7 daily. If the number of private vehicles remain constant during this period, then approximately only a third of vehicles will be HFCVs. On the other hand, considering HFC-REs, 38.5 million HFC-REs can potentially be supported at 90% capacity and full capacity, 43.9 million vehicles. Figure 5.1 shows the number of HFCVs, and HFC-REs supported by the best-case scenario separately. Investing in HFC-REs will reduce the need to build a substantial number of HRSs. However, further investments in electrical infrastructure will also be necessary to ensure sustainability. In terms of HFCVs, the hydrogen demand proposed in the best-case scenario cannot meet the required threshold for a complete transition to a hydrogen-based infrastructure.

According to the most extreme scenario proposed by Almansoori and Shah (2012) the hydrogen infrastructure can support 941000 HFCVs at maximum capacity or 3.14 million HFC-REs. The scenario proposed forecasted the growth for the year 2022. However, UK's official figures show approximately 4000 HFCVs in the UK (GOV.UK, 2019), suggesting that the UK is well behind in achieving the worst-case scenario, let alone any other one. One of the limitations of Almansoori and Shah's work is that it considered the growth of HBVs solely, yet the impact of other zero-emission vehicles will play a considerable role. It is unlikely that hydrogen will see a growth without a pushback from conventional vehicles by improved efficiencies and cleaner fuel blends.

The moderate scenario was determined by using the best-case scenario of Moreno-Benito et al. (2017). HFCVs will also displace approximately a fourth of conventional vehicles, as shown in figure 5.2. Here, the hydrogen demand was more conservative than that of Almansoori and Shah, and when utilised with HFCVs, the hydrogen demand projected only displaced approximately 6 million vehicles. However, if HFC-REs are pursued, then over two-thirds of conventional vehicles are replaced. Considerable investment and technological advancements are required for HFC-REs to become prominent.

The hydrogen demand estimated by the UKH2Mobility report is far more conservative than Almansoori and Shah or Moreno-Benito et al. (See figure 5.3 and table 5.5). According to the UKH2Mobility report, by 2030, 26.5 million conventional vehicles will still be on the road, with HFC-REs just exceeding 3.5 million. If manufacturers persist with HFCVs, only approximately 1.08 million vehicles will be on the roads by 2030. The UK's government has pledged to stop manufacturing full conventional vehicles from 2017, and so HBVs can play a greater role with a more aggressive strategy.

The UK can decarbonise its road transportation by combining hydrogen with other hybrids and EVs while offering a safer option to consumers. However, carbon emissions will still be emitted at the expense of road transportation due to the means and resources of hydrogen and electricity productions. Producing hydrogen from fossil-based fuels will only contain the issue until they become depleted. Hydrogen on its own is not the solution. Alternative options will have to be utilised to reduce the dependence on fossil fuels. This will extend the availability and usage of fossil fuels beyond 2050-2060 period until further progress is made. Investing in HFC-REs will also form part of the solution. Current UK efforts, as demonstrated above, are well short of achieving the worst-case scenario. A wider influx of funding and planning is required if hydrogen is to decarbonise the UK's road transportation and not simply replace the ICEVs and channel emissions produced down another route.

5.4.2 Near and long-term hydrogen projections

The projections made by Almansoori and Shah and the UKH2Mobility report covered 2005-2022 and 2015-2030, respectively. According to this, the projections made by Almansoori and Shah were overzealous for this period and are realistic for 2020-2060 with the necessary investment and push from all stakeholders including consumers. The UKH2Mobility report has projected approximately 65 small RS to be built by 2020, which is unlikely as currently, the UK has 18 stations. Unless the policy is changed substantially with significant investment to various stakeholders involved, such as ITM, this is also an ambitious projection. Moreno-Benito et al. projected a hydrogen demand of just over 25×10^6kg/year by 2025. This would require a network of 343 HRSs with a daily capacity of 200 kg/day or a network of 69 HRSs with a daily capacity of 1000kg/day to be built by 2025 to meet the demand. Larger stations must be built sooner rather than later to meet near-term projections.

In terms of long-term projections made for hydrogen, the UKH2Mobility report projected a yearly demand of 255.5×10^6 kg, whereas, for the same year Moreno-Benito et al projected 50.1×10^6kg. The number of HFCVs sustained by both are 983×10^3 and 1.93×10^5 at full capacity. The UK has approximately 30 million passenger vehicles, and this sector is still experiencing growth. The amount of HFCVs sustained in 2030 is insignificant concerning conventional vehicles. The hydrogen demand predicted varies between studies and the time considered. Currently, the UK sees a deficient growth in stations compared to what is required for hydrogen to make any real penetration. Undoubtedly, hydrogen plays a role, but for a serious commitment from all parties involved, defining the 'hydrogen space' is necessary. The results indicate that hydrogen deployed as a range extender to EVs will enjoy more success. Inevitably, fossil fuels will stop being employed as a transportation fuel in the future, and so non-FC hybrids will be replaced by hydrogen-based hybrids (HFC-REs). Therefore, it is more convenient to invest in HFC-REs with a more extensive centralised network.

5.4.3 Three hydrogen penetration scenarios

Three scenarios were developed, best-case, moderate-case, and extreme-case scenarios to analyse the HBV forecast for the UK. This will allow unrealistic scenarios to be eliminated and hence, incorporate the best-case strategy into the third-order model in chapter 6. Considering the extreme-case scenario, the number of HBVs sustained by the network by 2060 is negligible (figure 5.4). 5063 HBVs can be supported, half of which are HFCVs, and the other half consists of HFC-REs. This reflects the worst-case scenario for the UK, and efforts and policies favour NFC-EVs (Non-fuel cell hybrids and electric vehicles combined), resulting in the progress being made for hydrogen stalling.

Since a much greater level of investment is required for the moderate state, it is inevitable that hydrogen will employ a more attacking strategy. For this reason, the attack rate was increased, and so the number of conventional vehicles reduced corresponded to the growth of HBVs (figure 5.5). Furthermore, increasing investments and commitments from all stakeholders for the best-case scenario resulted in the attack rate being increased yet again. So, the number of

ICEVs reduced much in the same way as in the first two scenarios. The remaining ICEVs in the year 2060 will be removed from the road at the end of their lifecycle. The modelling assumed that HFCVs and HFC-REs would each grow according to the current 5% growth that the UK's road vehicles have endured at a 50:50 ratio. Suppose the ratio was altered in favour of HFC-REs with electricity playing a more significant role. In that case the number of HBVs will also increase at a greater rate to the decline of conventional vehicles.

If the UK decides to primarily on HFCVs or HFC-REs, the investment and development of the infrastructure will vary. For HFCVs, $8 \times 10^9 \text{kg}/H_2$ is required to maintain a fleet of HFCVs, whereas a fleet of HFC-REs only requires 2.5×10^9 kg/H_2 (see figure 5.7 and 5.8). In terms of the HFC-REs, the electrical infrastructure will also need to be developed prominantly to maintain the excess demand.

Manufacturers are pledging to stop manufacturing pure ICEVs (Motoring Research, 2021), so the current number of vehicles need to be replaced by the same number, if not more, to meet the additional demand of vehicles as growth continues. This is where HFC-REs can make a gap-bridging role. The EV charging infrastructure can play a significant role and eliminate the need to build many HRS.

Hydrogen has approximately 30 years to become the primary source of energy carrier for the transportation network, whereas utilising crude oil as the predominant source of energy took the best part of a century to evolve. Other energy carriers will substitute oil with a rough timeframe of 30-35 years. Policymakers and industry will determine the magnitude of hydrogen's role and how soon this transition will occur, considering energy security and future supply. Hydrogen's capability of meeting energy objectives suggests that it will have a considerable proportion of tomorrow's energy demand. However, how will the demand for hydrogen be met, and where will the energy of manufacturing hydrogen on a large scale come from, i.e. from renewable or non-renewable energy?

5.5 Conclusions and chapter summary

This chapter considered the introduction of hydrogen as a transportation fuel for passenger vehicles in the UK. The model proposed in chapter 4 was used to simulate different scenarios obtained from literature to evaluate the model developed against current SC proposals. From the results section, the model was able to simulate the different proposals across the timescale of 2020/2060, and if required, over the timescale proposed in the respected papers.

Three different proposals were selected covering a wide range of projections for the UK, such as conservative (UKH2Mobility, 2013), moderate (Moreno-Benito et al., 2017), and optimistic (Almansoori and Shah, 2012) projections. The UK's current level of investment is minimal in line with the UKH2Mobility report. If the investment for hydrogen follows this route, then hydrogen will not play a significant role in tomorrow's passenger vehicle fleet. The UK's current progress is near the most extreme scenarios proposed by Almansoori and Shah (2012) as well as Moreno-Benito et al (2017). The UkH2Mobility report expects a sizeable infrastructure in place by 2030, which can support 1.18 million or 3.92 million HFC-REs. This only covers 3.93% or 13.1% of the passenger vehicle fleet operating at maximum capacity. A greater influx of investment and growth in this sector is required before HBVs can become competitive with conventional vehicles.

Furthermore, this case study assumed that the upper limit for hydrogen is if the entire private fleet was replaced by HBVs, however current analysis suggests that conversion of half the private fleet is overzealous. Therefore, it is improbable that a complete transition to hydrogen will occur. Furthermore, the model investigated the role of hydrogen and conventional vehicles. However, several vehicle types competing with conventional such as EVs, and hybrids. The model proposed in chapter 4 is extended to a third order model to allow multiple AFVs to compete with conventional ones to overcome these limitations. Hydrogen penetration scenarios are also limited to 50% of the private vehicle fleet.

Chapter 6: Third order model and optimisation results

6.1 Introduction

The UK's vehicle fleet constitutes of several different vehicle types. This chapter explores the dynamic behaviour of three categories: conventional vehicles, hydrogen-based vehicles, and non-fuel cell hybrids combined with pure electric vehicles. As demonstrated in chapters 4 and 5, the introduction of hydrogen-based vehicles can be analysed by utilising the second-order model. It is interesting to extend the previous work to capture the interactions of different technologies in the private vehicle sector by introducing the third-order model. There are three variants of the third-order model, namely, M1, M2, and M3, corresponding to 2 Predators – 1 Prey; 2 Predators – 2 Prey; and 2 Predators – 3 Prey. The most suitable model representing the UK's passenger vehicle market is considered as determined by policies. This is then used to assess the most suitable scenarios before optimisation in terms of fuel economy and emissions. The optimisation is carried out using the linear – quadratic regulator optimal techniques.

6.2 The extended third state Lotka-Volterra Model

6.2.1 Model Description

The third-order model is an extension of the second-order model to incorporate multiple interacting passenger vehicle types. This allows more realistic scenarios representing the UK's passenger vehicle market to be simulated. Three cyclical species have been considered in a number of papers, such as (Filho et al., 2005; Hsu et al., 2015). Three variants of the third-order model were proposed in terms of prey and predators based on literature and current investment and pledges by the government (see figure 6.1).

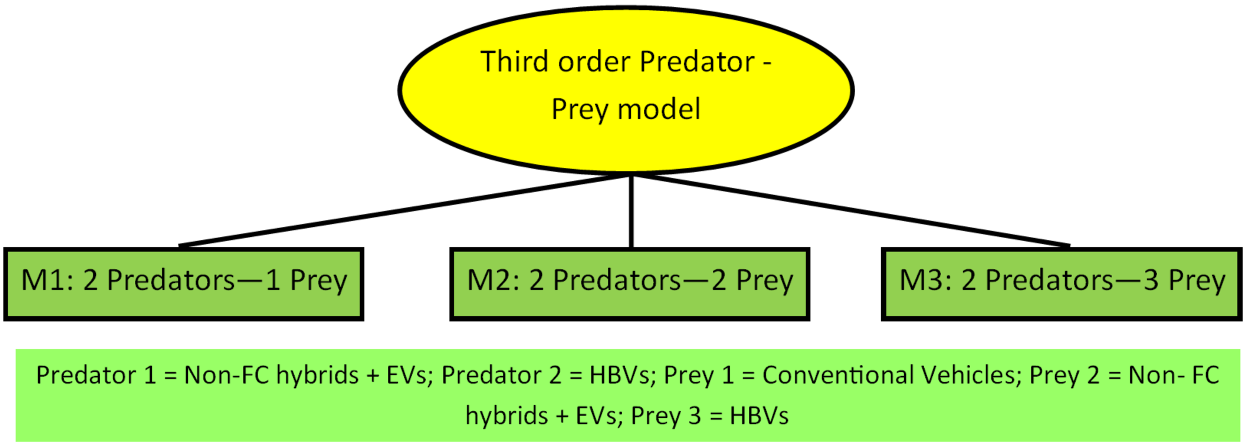


Figure 6. 1: Overview of the third order models

Currently, the UK is investing in low carbon energy sources for road transportation with different policies and incentives in place for technologies competing in the private vehicle sector (GOV.UK, 2014a, 2016, 2018a). These policies will determine the type of role and competitiveness of each technology with respect to others. Currently, EVs and non-FC hybrids (NFC-EVs) have most of the funding, alongside vehicles and infrastructure in place compared to others. It is difficult to consider the impact of policies and future legislation, funding, and shareholder opportunities into account without allocating arbitrary values as exogenous parameters to the model or to the demand input. However, the benefit of the predator-prey model is that these can be considered by adjusting some of the parameters, such as the attack rate or conversion rate, by incorporating a percentage for these factors.

Since there are three groups of fuel technologies under consideration here, three versions of the model, namely, M1, M2, and M3 (see figure 6.1), have been developed to encompass the interaction between the three groups of technology. If the emphasis is placed on reducing the reliance on fossil fuels and GHG emissions, then it is proposed that alternative fuel technologies will not compete against each other, but against conventional vehicles. Both the predators, in this case, NFC-EVs and hydrogen-based vehicles (HBV) will attack conventional vehicles – the sole prey. This situation is represented in the M1 model. So, in other words, conventional vehicles will see a growth, which is then affected by the growth of NFC-EVs and HBVs. However, the number of conventional vehicles displaced will depend on the attack and conversion rates that are influenced by the strength of policies and investment into the technology.

The M2 model is proposed where HBVs will act as a predator to both conventional vehicles and NFC-EVs. This will help drive HBVs forward as the NFC-EVs will only predate on conventional vehicles. Here, it is envisaged that the HBVs are attacking the ICE of the non-FC hybrids. New technologies introduced into a market will compete against other new technologies as well as more traditional ones facing common barriers such as high cost, low consumer knowledge, and low-risk tolerance by potential adopters (Hardman et al., 2017b). The severity of the attack rate of HBVs will be adjusted by the attack rate depending on the strategy deployed. If the government pledges an increase in spending for HBVs and corresponding infrastructure, then the attack rate will also be increased.

Furthermore, the already established NFC-EVs will also significantly reduce the impact of HBVs. So, therefore, it is sensible to assume that both predators will attack each other as well as conventional vehicles. Conventional vehicles, however, will not predate at all as they will not make a comeback once eradicated. This is due to conventional fuel being non-renewable with limited reserves, and devastating environmental impact. This has led to the M3 model, where all vehicle types will attack except for conventional ones.

The most realistic model will be linearised so that the various strategies can be optimised using Linear-quadratic regulator (LQR) optimal techniques considering the stability of the system (Purnawan et al., 2017; Dul et al., 2020). The LQR control synthesises the feedback control (Kemper et al., 2013).

$$\boldsymbol{u = -Kx} \qquad \text{Equation 6. 1}$$

Where x and u are state and control vectors, and K is the gain matrix. The aim here is to find the optimal control u by minimising the Quadratic Performance Index (J) (Equation 6.2):

$$\text{Min u(t)} \qquad \boldsymbol{J(x(t), u(t)) = \int_0^{\infty} (x^T(t) Q x(t) + u^T(t) R u(t)) dt} \qquad \text{Equation 6. 2}$$

J is a quadratic measure of future behaviour (Kemper et al., 2013), and the origin or a different value can be used as the target of this behaviour. Q ≥ 0, and R > 0, symmetric, positive (semi) definite weighting matrices (Murray, 2006) for state and control. The Q term designates the deviation of states from the target implicitly measuring convergence rate (rise time and settling), whereas the R term signifies the penalisation of the aggressive use of the input, i.e. the amount of control. Squares are used because they tend to provide easier analysis and well-behaved solutions that are relatively insensitive to changes in initial conditions. The constraints of J are provided by the linear state model:

$$\begin{gathered} \boldsymbol{\dot{x}(t) = Ax(t) + Bu(t) \ and \ y = Cx + Du,} \\ \boldsymbol{x(t_0) = x_0, \ x \in R^n, \ u \in R^n} \end{gathered} \qquad \text{Equation 6. 3}$$

The steady-state model of the system consists of two system equations. The system or state matrix A and B is the control matrix. The second equation consists of C as the output matrix and D, the direct transition of the feed-forward matrix (Ajasa and Sebiotimo, 2014). In LQR control, a linear system is required without disturbances where the time scope is large. As a result of these assumptions, a solution in a closed loop can be determined by solving the algebraic Riccati matrix Equation (ARE):

$$\boldsymbol{A^T P + PA - PBR^{-1} B^T P + q = 0} \qquad \text{Equation 6. 4}$$

The stabilising solution, P, is > 0 and used to gain the matrix K (Dul et al., 2020):

$$\boldsymbol{K = R^{-1}B^{T}P} \qquad \text{Equation 6. 5}$$

The key decision in the design of optimal controller using LQR is the choice of Q and R matrices in that these are often the trade-offs between input activity and rates of convergence (Nagarkar et al., 2018). The success of using LQR largely ends on the selection and tuning of Q and R because there is no established method of selecting them (Dul et al., 2020). The simplest way is to set Q as the identity matrix whilst adjusting the R-value through trial and error (on weights) to find the optimal solution (Murray, 2006).

6.2.2 Policies

The policies outlined in sections 3.2.2 and 4.2.2 are also considered alongside the following:

Policy 1 (P6.1): The government has set targets for at least 50%, and potentially as many as 70% of new car sales to be electric vehicles by 2030 (Committee on Climate Change, 2019).

6.2.3 Assumptions

The third-order model has been modified to take on the roles of different interactions between the competitors. The assumptions made in this section are outlined below:

Assumption 1 (A6.1): Conventional vehicles will only assume the role of prey in all three third-order models in line with P3.1, P3.2, P4.1, P4.2, and P6.1.

Assumption 2 (A6.2): NFC-EVs are collated to act as predator 1 and all HBVs are collated to act as predator 2. Every NFC-EV introduced to the market will replace 1 ICEV for all three cases, according to P6.1.

Assumption 3 (A6.3): The two predators will compete to replace the conventional vehicles only and will not interact with each other in the M1 model in line with P3.1.

Assumption 4 (A6.4): NFC-EVs will also behave both as prey and predator in the case of the M2 model: they will predate on conventional vehicles but attacked by HBVs with respect to P3.4.

Assumption 5 (A6.5): NFC-EVs will attack both conventional vehicles and HBVs in the M3 model but only attacked by HBVs.

Assumption 6 (A6.6): HBVs will assume both roles too: they will predate on conventional in all three cases, attacked by NFC-EVs in M3 model, while attacking NFC-EVs in both the M2 and M3 models. The attack rate of HBVs on conventional vehicles will replace a third of conventional in the extreme scenario. For the moderate case, for every 2 HBVs introduced, one ICEV will be replaced, and for the best-case scenario for every HBV introduced, one conventional will be removed.

Assumption 7 (A6.7): The HBVs will consist of an equal number of HFCVs and HFC-REs in all three models.

Assumption 8 (A6.8): Since NFC-EVs rely on the grid, i.e. electricity produced primarily from fossil fuels and can be charged at home as well as recharge points. It will be assumed that the efficiency will be 100% as surplus electricity will be used for other applications via the grid, and shortage of electricity can be recharged at home or recovered depending on the hybrid type and hybrid technology utilised.

6.2.4 Governing Equations

This section consists of the governing equations covering the three types of third-order models. The model was extended to include a third variable/input representing hybrid vehicles from the results depicted by the second-order model. The third-order models will be used to analyse the road transportation space before narrowing it down to the range-extender space.

6.2.4.1 M1 Model

The third-order model consists of three parameters (figure 6.2), namely, prey (conventional), first predator (NFC-EV) and the second predator (HBV). The second-order equations are manipulated to represent the two predators. The single prey equation of the third-order system in generic form (equation 6.6) and is an extension of equation 4.1:

$$\boldsymbol{\dot{x}_1 = x_1(-a + bx_2 + ex_3) + \mu_1} \qquad \text{Equation 6. 6}$$

a is the growth rate of ICEVs, and b is the attack rate of NFC-EVs on ICEVs. Here, an additional term was included representing the second predator in x_3, and e represents the attack rate on ICEV i.e. the displacement of ICEV by HBVs. HBVs, in this case represents all hydrogen vehicles (full + range extenders). The $\boldsymbol{\mu_1}$ reflects the total conventional fuel input for one year. The two predator equations will only consist of two terms since they do not interact with each other so are essentially two-state equations. The first predator equation of the third order model:

$$\dot{\boldsymbol{x}}_2 = \boldsymbol{x_2}(\boldsymbol{d} + \boldsymbol{c}\boldsymbol{x_1}) + \boldsymbol{\mu_2} \qquad \text{Equation 6. 7}$$

The second equation (equation 6.7) representing the predator 1 as x_2 remains the same as the second-order one and only interacts with the prey. In this case d is the growth of NFC-EVs, c is the conversion efficiency of ICEVS into HBVs, and $\boldsymbol{\mu_2}$ is the total fuel input for NFC-EVs. The second predator equation of the third-order model:

$$\dot{\boldsymbol{x}}_3 = \boldsymbol{x_3}(\boldsymbol{g} + \boldsymbol{h}\boldsymbol{x_1}) + \boldsymbol{\mu_3} \qquad \text{Equation 6. 8}$$

The third equation represents (equation 6.8) predator 2 in the form of x_3 but only interacts with the prey. Here, g represents the growth of HBVs, h is the hydrogen efficiency and $\boldsymbol{\mu_3}$ is the total fuel input for HBVs.

6.2.4.2 M2 Model

Here, in the first equation, the prey will remain the same as in section 6.2.4.1 and conventional vehicles will only assume the role of prey and be attacked by both the predators (figure 6.3). In this case, the first predator will encompass a third term which represents the attack rate of the second predator. Equation 6.9 represents the first predator of the third-order model encompassing the attack rate of the second predator.

$$\dot{\boldsymbol{x}}_2 = \boldsymbol{x_2}(\boldsymbol{d} + \boldsymbol{c}\boldsymbol{x_1} - \boldsymbol{f}\boldsymbol{x_3}) + \boldsymbol{\mu_2} \qquad \text{Equation 6. 9}$$

The second equation representing the HFC-RE as x_2 has also been extended. Here, x_3 represents the number of HBVs available per year, and f is the attack rate of HBVs on NFC-EVs. The third equation representing predator 2 will remain the same as in section 6.2.4.1, since NFC-EVs will not be attacking HBVs.

6.2.4.3 M3 Model

In this case, both the conventional equation will remain same as the one in section 6.2.4.1 (equation 6.6) and the predator 1 equation will remain the same as sections 6.2.4.2 (equation 6.9). This time the third equation will be modified to encompass the attack rate of NFC-EVs (figure 6.4). The final equation (equation 6.10) of the third-order model:

$$\dot{\boldsymbol{x}}_3 = \boldsymbol{x_3}(\boldsymbol{g} + \boldsymbol{h}\boldsymbol{x_1} - \boldsymbol{i}\boldsymbol{x_2}) + \boldsymbol{\mu_3} \qquad \text{Equation 6. 10}$$

For the HBVs, g is the growth rate of HBVs i.e. rate of increase per unit time, h is the efficiency of the number of HBVs displace conventional ones, and I represents the attack rate NFC-EVs on HBVs.

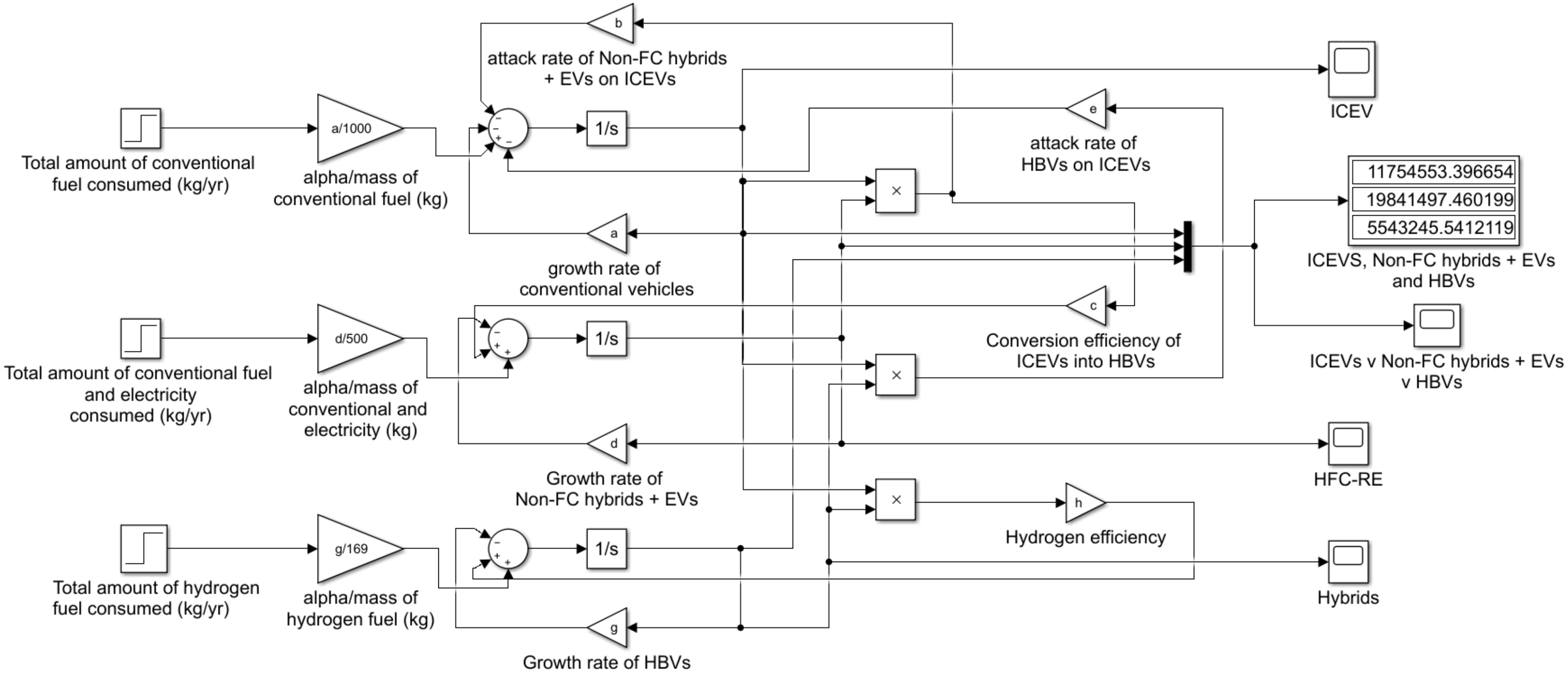


Figure 6. 2: Block diagram representing the M1 model.

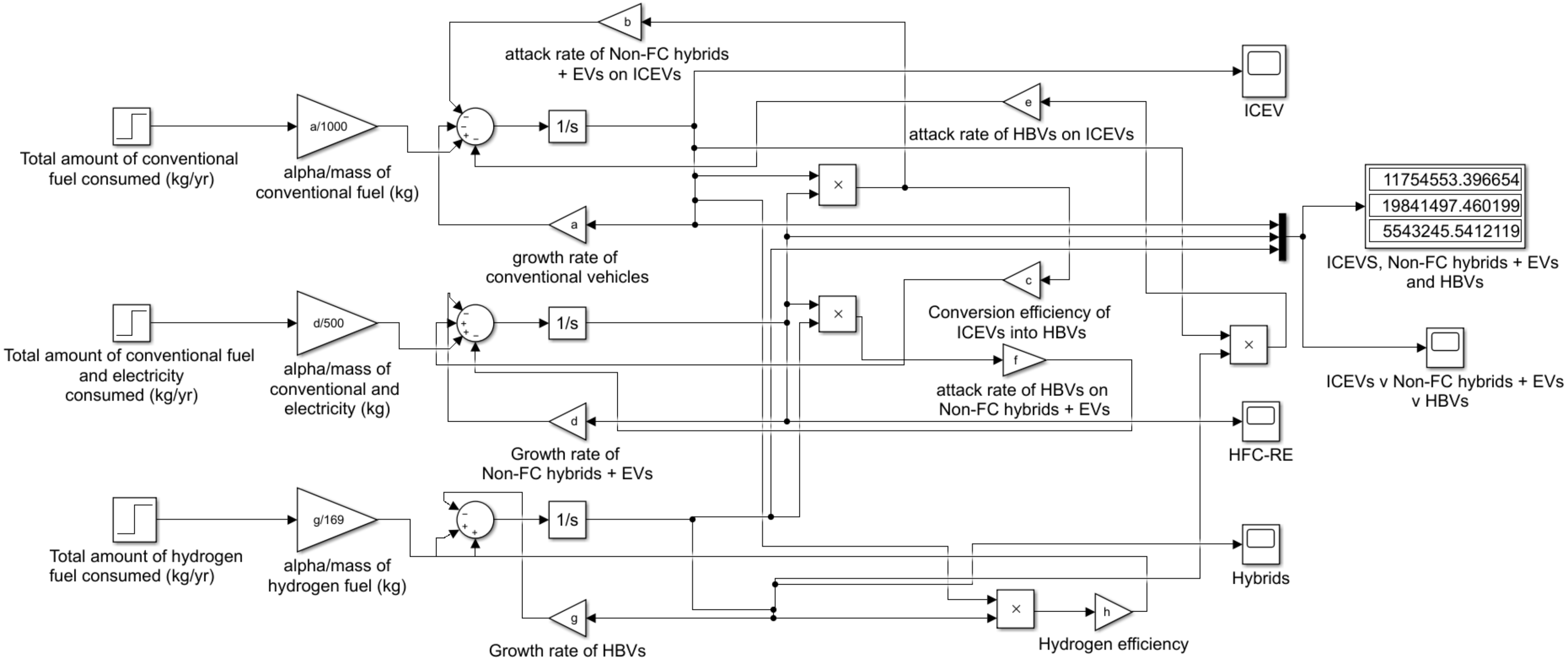


Figure 6. 3: Represents the Simulink model of the M2 model.

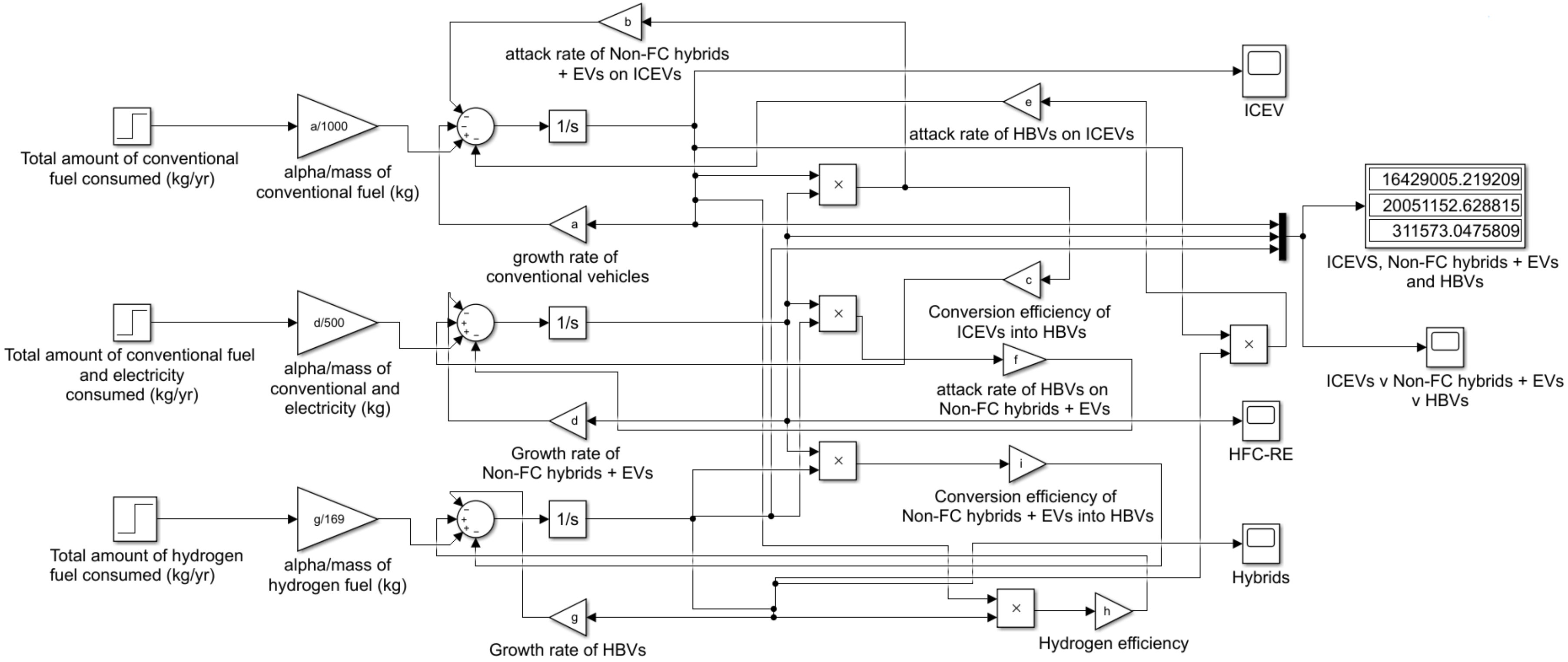


Figure 6. 4: Simulink block diagram representing the M3 model.

6.2.5 HRS efficiencies

The size of the HRS network depends on the number of HBVs on the road, the capacity of each station and its operating level (see table 6.1). Some studies have assessed HRS at 100% efficiencies to see how well the model works (Forsberg and Karlström, 2007; Siyal et al., 2015). A study conducted in Sweden considered the operation of HRS to meet the required hydrogen demand, and so, in other words, the unmet load of the RS was set at 0%. The hydrogen load profile was varied, demonstrating peak times between 8-9 am and 5-6 pm alongside minimum demand during night and early morning (Siyal et al., 2015). Operating at maximum efficiency (100%) was used as the benchmark here to compare the different models and finding the optimum number of stations required. The number of refuelling stations (RSs) in the UK has been on a steady decline from 13107 in 2000 to 8385 in 2019 (statista, 2020). This indicates that current RSs operate closer to the maximum capacity of each station. A similar trend can be expected with HRSs, hence the selection of 75% efficiency.

Table 6. 1: Definitions of the HRS operating efficiencies selected for the third order models.

HRS operating efficiencies (%)	Definition	References
100	HRSs are operating at maximum capacity	(Siyal et al., 2015; Forsberg and Karlström, 2007)
75	HRSs are operating at 75% of their capacity – excess is either stored or production is decreased.	(Grüger et al., 2018)
50	HRSs are operating at half their capacity	
25	HRSs are operating at 25% of their capacity – Stations are largely under-utilised and expensive to maintain	(Proost and Vanhoof, 2015)

In a different study, it was assumed that the different size stations dispensed between 70-80% of hydrogen in kg/day (Grüger et al., 2018). So therefore, 75% operating efficiency was considered alongside maximum utilisation. In much of the literature, it is considered that HRS will initially be under-utilised, especially in the pre-commercialisation phase (Wyllie, 2018). For this reason, both 50% and 25% utilisation were considered. In a different study, Talebian et al. (2019) considered the HRS to operate at maximum capacity as the upper limit and 10% of the maximum capacity for the lower limit.

6.2.6 Model Simulation

In this section, the third-order model presented in the above sections was used to evaluate the effectiveness of introducing HFCVs into the road transport sector while NFC-EVs have already penetrated. The three penetration strategies from the second-order model consisting of extreme, moderate, and best-case scenarios were repeated. Table 6.2 represents the definitions of the parameters used in M1, M2, and M3 models. Parameters a, b, c, d, e, and h are consistent for all three models. The parameter f, the attack rate of HBVs on NFC-REs, is applicable to third order models consisting of M2 and M3. Parameter I, the conversion efficiency of NFC-REs, is applicable to the M3 only.

Table 6. 2: Definitions of the parameters used in the third order models.

Parameter	Definition	Explanation
a	Growth rate of conventional vehicles (ICEVs)	5% based on literature
b	Attack rate of NFC-EVs on ICEVs	The attack rate will remain constant as hybrids are effectively replacing conventional vehicles in the market.
c	Conversion efficiency of ICEVs into HBVs	Conversion efficiency depends on how successful the conversion is from ICEV to a HBV one and this is also scenario dependent.
d	Growth rate of NFC-EVs	The growth rate of NFC-EVs is also set to 5% for all predators following the UK's vehicle growth rate over the last 50 years.
e	Attack rate of HBVs on ICEVs	Attack rate depends on the scenario i.e. for the extreme scenario the attack rate will be low
f	Attack rate of HBVs on NFC-EVs	Attack rate depends on the scenario i.e. for the extreme scenario the attack rate will be low
g	Growth rate of HBVs	The growth rate of HBVs is also set to 5% for all predators following the UK's vehicle growth rate over the last 50 years.
h	Hydrogen efficiency	Hydrogen Efficiency is modified according to the scenario and the percentage of HRS being utilised. Maximum utilisation of 100% is set as the benchmark.

i	Conversion efficiency of NFC-EVs	Conversion efficiency depends on how successful the conversion is from NFC-EVs to a HBV one and this is also scenario dependent.

Table 6.3 provides the magnitude of each parameter considering three scenarios, namely, extreme, moderate, and best-case. Most of the parameters were calculated from the model developed. Hydrogen efficiency at a growth of 5% can achieve 100, 90 and 86.5% efficiencies for HRS utilisation. Lower levels of operations can only be derived by the model if the attack rate is also lowered. So, the 5% growth is the upper bound as conventional vehicles have seen the same growth. Hydrogen efficiency parameters are outlined in table 6.4.

Table 6. 3: The parameters used in the three third order models for extreme, moderate, and best-case scenarios.

Parameter	Definition	Extreme	Moderate	Best case
a	Growth rate of conventional vehicles (ICEVs)	0.05	0.05	0.05
b	Attack rate of NFC-EVs on ICEVs	2.2e-9	2.2e-9	2.2e-9
		1	1	1
c	NFC-EVs efficiency	1.818e-10	1.818e-10	1.818e-10
		100%		
d	Growth rate of NFC-EVs	0.05	0.05	0.05
e	Attack rate of HBVs on ICEVs	6.9e-10	3e-9	2.3e-8
		0.25	0.5	0.8
f	Attack rate of HBVs on NFC-EVs	0.45e-9	1.025e-9	5e-9
		0.001	0.1	0.4
g	Growth rate of HBVs	0.05	0.05	0.05
i	Attack rate of NFC-EVs on HBVs	4.5e-8	4.5e-8	4.5e-8
		1	1	1

Six scenarios were selected to evaluate the effectiveness of the models. The first scenario displays the case where both NFC-EVs and HBVs fail to penetration the market beyond pre-commercialisation or early adopters. The second scenario displays the case where NFC-EVs manage to successfully attain approximately 50% share of the market with HBVs stalling at pre-commercialisation. The third scenario depicts the reverse of scenario 2 where HBVs manage to attain approximately 50% of the market share and NFC-EVs stall after initial success. The fourth scenario demonstrates that NFC-EVs become the dominant vehicle type with scenario 5 showing the reverse of this where HBVs become dominant. Finally, the sixth scenario shows that both NFC-EVs and HBVs moderately share majority of the market.

Table 6. 4: The variation in the h parameter of hydrogen efficiency in terms of growth rate.

Parameter	Definition	Growth rate
h	Hydrogen efficiency	3.45e-10 at 5% growth
		100%
		9.75e-11 at 5% growth
		90%
		9.75e-13 at 5% growth
		86.5%
		5.5e-12 at 0.04 growth rate
		80%
		14.63e-11 at 3% growth
		75%
		3.8e-12 at growth of 3%
		70%
		1.65e-10 at a growth of 2%
		60%
		7.033e-10 at 1% growth rate
		50%
		3.385e-10 at 1% growth rate
		40%
		1.075e-10 at 1% growth rate
		35%
		8.15e-10 at 0.5% growth
		30%
		5.353e-10 at 0.5% growth rate
		25%

In terms of the market proportion of HBVs, the maximum proportion of market share will be capped at 50%. Current policies and investment are strongly in favour of hybrids and EVs (HM Government, 2018; DfT, 2020). The lower limit is taken at 20% because of the advantages of HBVs in terms of refuelling time and range (Campíñez-Romero et al., 2018b). Table 6.5 below outlines the parameters used in the 4 scenarios selected based on market share. Further considerations include the level of capacity utilised per RS.

Table 6. 5: Parameters considered in different scenarios with consideration to the market share of the predators.

Scenario	Proportion of NFC-EVs: HBVs	Fuel Input NFC-EVs: HBVs	RS utilisation (%) (NFC-EVs: HBVs)
1	80:20	12.8e9: 1.082e9	100: 100, 75, 50, 25
2	70:30	11.2e9: 1.923e9	
3	60:40	9.6e9: 2.164e9	
4	50:50	8e9: 2.704e9	

As mentioned in section 6.2.5, four levels of HRS utilisation are considered: 100%, 75%, 50% and 25%. So, for each scenario depicted, the HRS efficiency will be varied for hydrogen. For NFC-EVs, the RSs are taken to operate at 100% since the vehicles can be charged at home using the national grid or at a service recharge point.

6.2.7 Linearisation of the Model

Optimisation of the third state model is carried out in this section. The model is linearised around the steady state so that it can be optimised using the LQR optimal techniques. The M3 model is presented below:

$$\dot{x}_1 = x_1(-a + bx_2 + ex_3) + \mu_1 \quad \text{Equation 6. 11}$$

$$\dot{x}_2 = x_2(d + cx_1 - fx_3) + \mu_2 \quad \text{Equation 6. 12}$$

$$\dot{x}_3 = x_3(g + hx_1 - ix_2) + \mu_3 \quad \text{Equation 6. 13}$$

At steady state,

$$\frac{dx}{dt} = 0 \quad \text{Equation 6. 14}$$

Hence, the third- order equations here were equated to 0 as the first equilibrium point is determined when the system is at 0.

$$-ax_1 + bx_1x_2 + ex_1x_3 + \mu_1 = 0 \qquad \text{Equation 6. 15}$$

$$dx_2 + cx_1x_2 - fx_2x_3 + \mu_2 = 0 \qquad \text{Equation 6. 16}$$

$$gx_3 + hx_1x_3 - ix_2x_3 + \mu_3 = 0 \qquad \text{Equation 6. 17}$$

The three equations are then rearranged to make the respected fuel inputs the subjects.

$$\mu_1 = ax_1 - bx_1x_2 - ex_1x_3 \qquad \text{Equation 6. 18}$$

$$\mu_2 = -dx_2 - cx_1x_2 + fx_2x_3 \qquad \text{Equation 6. 19}$$

$$\mu_3 = -gx_3 - hx_1x_3 + ix_2x_3 \qquad \text{Equation 6. 20}$$

The initial conditions of the system are $x_1^0, x_2^0, x_3^0, \mu_1^0, \mu_2^0, and\ \mu_3^0$. The equations are then modified as shown below in encompass change using the product rule. Modification of the equations using the product rule:

$$\Delta\dot{x}_1 = -a\Delta x_1 + b\Delta(x_1x_2) + e\Delta(x_1x_3) + \Delta\mu_1 \qquad \text{Equation 6. 21}$$

$$\Delta\dot{x}_2 = d\Delta x_2 + c\Delta(x_1x_2) - f\Delta(x_2x_3) + \Delta\mu_2 \qquad \text{Equation 6. 22}$$

$$\Delta\dot{x}_3 = g\Delta x_3 + h\Delta(x_1x_3) - i\Delta(x_2x_3) + \Delta\mu_3 \qquad \text{Equation 6. 23}$$

The equations are then expanded before like terms are collated:

$$\Delta\dot{x}_1 = -a\Delta x_1 + bx_2^0\Delta x_1 + bx_1^0\Delta x_2 + ex_3^0\Delta x_1 + ex_1^0\Delta x_3 + \Delta\mu_1 \qquad \text{Equation 6. 24}$$

$$\Delta\dot{x}_2 = d\Delta x_2 + cx_2^0\Delta x_1 + cx_1^0\Delta x_2 - fx_3^0\Delta x_2 - fx_2^0\Delta x_3 + \Delta\mu_2 \qquad \text{Equation 6. 25}$$

$$\Delta\dot{x}_3 = g\Delta x_3 + hx_3^0\Delta x_1 + hx_1^0\Delta x_3 - ix_3^0\Delta x_2 - ix_2^0\Delta x_3 + \Delta\mu_3 \qquad \text{Equation 6. 26}$$

Rearranging for like terms:

$$\Delta\dot{x}_1 = \Delta x_1\left(-a + bx_2^0 + ex_3^0\right) + bx_1^0\Delta x_2 + ex_1^0\Delta x_3 + \Delta\mu_1 \qquad \text{Equation 6. 27}$$

$$\Delta\dot{x}_2 = cx_2^0\Delta x_1 + \Delta x_2\left(d + cx_1^0 - fx_3^0\right) - fx_2^0\Delta x_3 + \Delta\mu_2 \qquad \text{Equation 6. 28}$$

$$\Delta\dot{x}_3 = hx_3^0\Delta x_1 - ix_3^0\Delta x_2 + \Delta x_3\left(g + hx_1^0 - ix_2^0\right) + \Delta\mu_3 \qquad \text{Equation 6. 29}$$

The three state equations are finally rearranged into the matrix form as presented below:

$$\begin{bmatrix} \Delta\dot{x}_1 \\ \Delta\dot{x}_2 \\ \Delta\dot{x}_3 \end{bmatrix} = \begin{bmatrix} -a + bx_2^0 + ex_3^0 & bx_1^0 & ex_1^0 \\ cx_2^0 & d + cx_1^0 - fx_3^0 & -fx_2^0 \\ hx_3^0 & -ix_3^0 & g + hx_1^0 - ix_2^0 \end{bmatrix} . \begin{bmatrix} \Delta x_1 \\ \Delta x_2 \\ \Delta x_3 \end{bmatrix} + \begin{bmatrix} \Delta\mu_1 \\ \Delta\mu_2 \\ \Delta\mu_3 \end{bmatrix}$$

The linearised third order model was developed in MATLAB Simulink. The linearised model will be optimised using LQR techniques in MATLAB Simulink as demonstrated in the following section with manipulation of the fuel input used to control the market. The scarcity of conventional fuel, limited supply of hydrogen will "force" the transition from a conventional non-renewable transport fuel.

6.2.8 Optimisation

The LQR controller was used to stabilise and optimise the third-order M3 model. Figure 6.5 shows the model developed in Simulink.

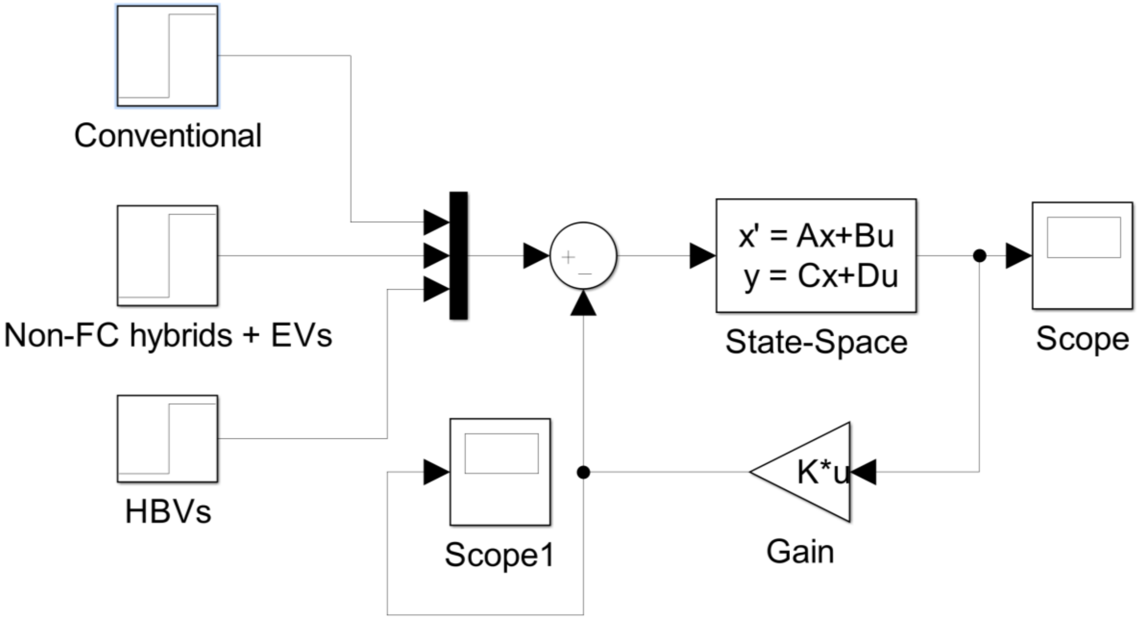


Figure 6. 5: Optimised model of the M3 model.

The choices of Q and R allows trade-offs between input activity i.e. number of vehicles, and rates of convergence i.e. fuel. Q will be assumed as the identity matrix (I), and R will be a multiple of the identity matrix initially, and trial and error will be used to find the optimal solution (Kumar et al., 2016; Dul et al., 2020). In this case, decarbonisation of the private vehicle fleet is the priority at the earliest opportunity, while issuing penalties on emissions. The PI is optimised considering fuel economy and emissions (Nagarkar et al., 2018).

Table 6. 6: The parameters selected for the optimisation approach.

Parameter	Definition in MATLAB Simulink	Definition
A	[-a+b*x2+e*x3 b*x1 e*x1; c*x2 -d+c*x1-f*x3 -f*x2; h*x3 -i*x3 g+h*x1-i*x2]	The system (Ajasa and Sebiotimo, 2014)
B	eye(3)	Input matrix (Ajasa and Sebiotimo, 2014)
C	eye(3)	Output matrix (Ajasa and Sebiotimo, 2014)
D	zeros(3,3)	Direct transition or feed-forward matrix (Ajasa and Sebiotimo, 2014)
Initial conditions	[0.3e6; -109973; -7307]	Selected pertaining to scenario
Q	Identity Matrix	Relative weight of state deviation
R	P x Identity Matrix	Relative weight of control

6.3 Results

6.3.1 Comparison of the models

In this section, the three variants of the third-order model were compared to assess the behaviour of the models under the same scenarios. Three penetration strategies were selected: extreme, moderate, and the best-case with a total of 6 scenarios. The scenarios represented the quantity of hydrogen fuel available in the infrastructure for the purpose of HFCVs. The penetration strategies further represented the influence of external factors on the growth of HFCVs. So, even with investment into the infrastructure, political or geographic factors can still potentially influence the uptake and growth of vehicles, such as more emphasis on public transport (HS2, 2022) and cycle initiatives (Environment, 2017).

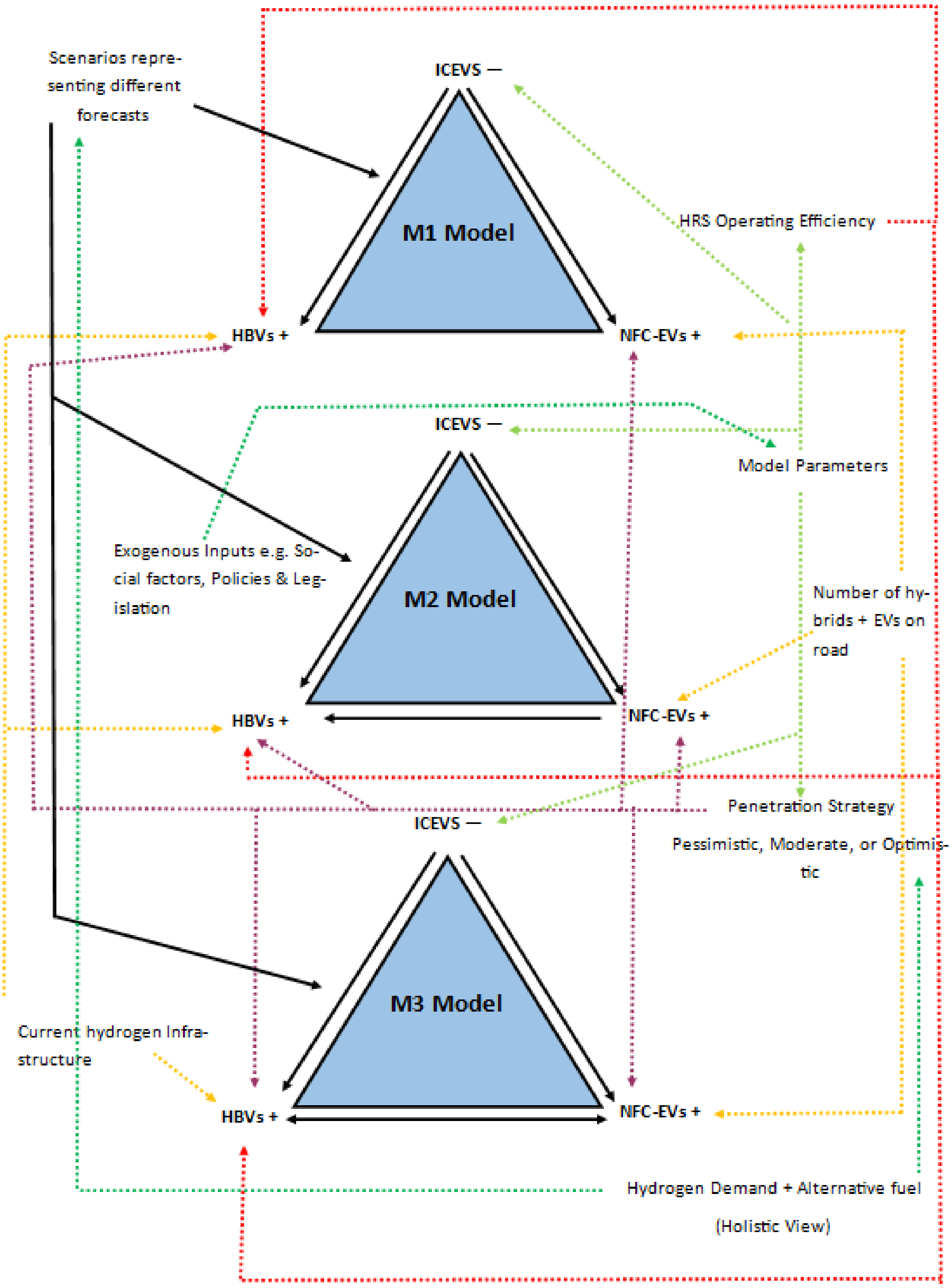


Figure 6. 6: An overview of the third order models representing the input and outputs of various parameters.

The fuel input for conventional vehicles was kept the same throughout, and the fuel input for NFC-EVs and HBVs were manipulated depending on the scenario. The reason conventional fuel was kept constant because it is the amount of fuel that the infrastructure has available and the capacity to provide if required. That is not the case with alternative fuel. Tables A.1, A.2 and A.3 in the appendices demonstrate the different scenarios using the M1, M2, and M3 models respectively. The results here were simulated assuming that HRS are operating at 100% efficiency. The results obtained from the three Models, while keeping all the parameters constant apart from the level of interaction between the competing fuels. The results pertaining to M2 demonstrate the predation of HBVs on both conventional and NFC-EVs. Current policies favour EVs and NFC-REs, so therefore, HBVs are competing within other AFVs. The impact of policies is considered via the models mutually interaction between the technologies. The results from M3 depict the policies and investment of both NFC-REs and HBVs.

The simulations from all three models are grouped in terms of scenario to visually demonstrate the behaviour of the models. Figure 6.7 shows the simulations obtained for scenario 1 for all the third-order models. For the extreme case, both NFC-EVs and HBVs attain a negligible proportion of the market with little impact on conventional vehicles because the level of investment was minimal, and policies were lenient to conventional vehicles. However, from figure 6.7 HBVs are seen to have no effect on the number of NFC-EVs using the extreme penetration strategy. On the other hand, the attack of NFC-EVs on HBVs does reduce the number of HBVs as seen in the M3 model. So, in other words, HBVs and NFC-EVs do not penetrate the vehicle market beyond pre-commercialisation and/or early adoption. This is because scenario 1 uses the extreme penetration strategy, and as a result, a negligible number of vehicles were supported by the infrastructure, and conventional vehicles remained dominant. Many studies in the literature proposed scenarios where the market penetration of hydrogen was 15% or under (Lahnaoui et al., 2018; Woo et al., 2016), suggesting that other vehicle types will also contribute to the sector. It is possible that the role of conventional vehicles will be prolonged as much as possible with improvements in technology, and efficiency whilst initiating better use and investment into public transport, such as High Speed Rail 2 (HS2, 2022), and hydrogen buses in Birmingham (Mavrokefalidis, 2020). These schemes will remove the number of journeys made by drivers, reducing the overall reliance on fossil fuels extending their lifetime.

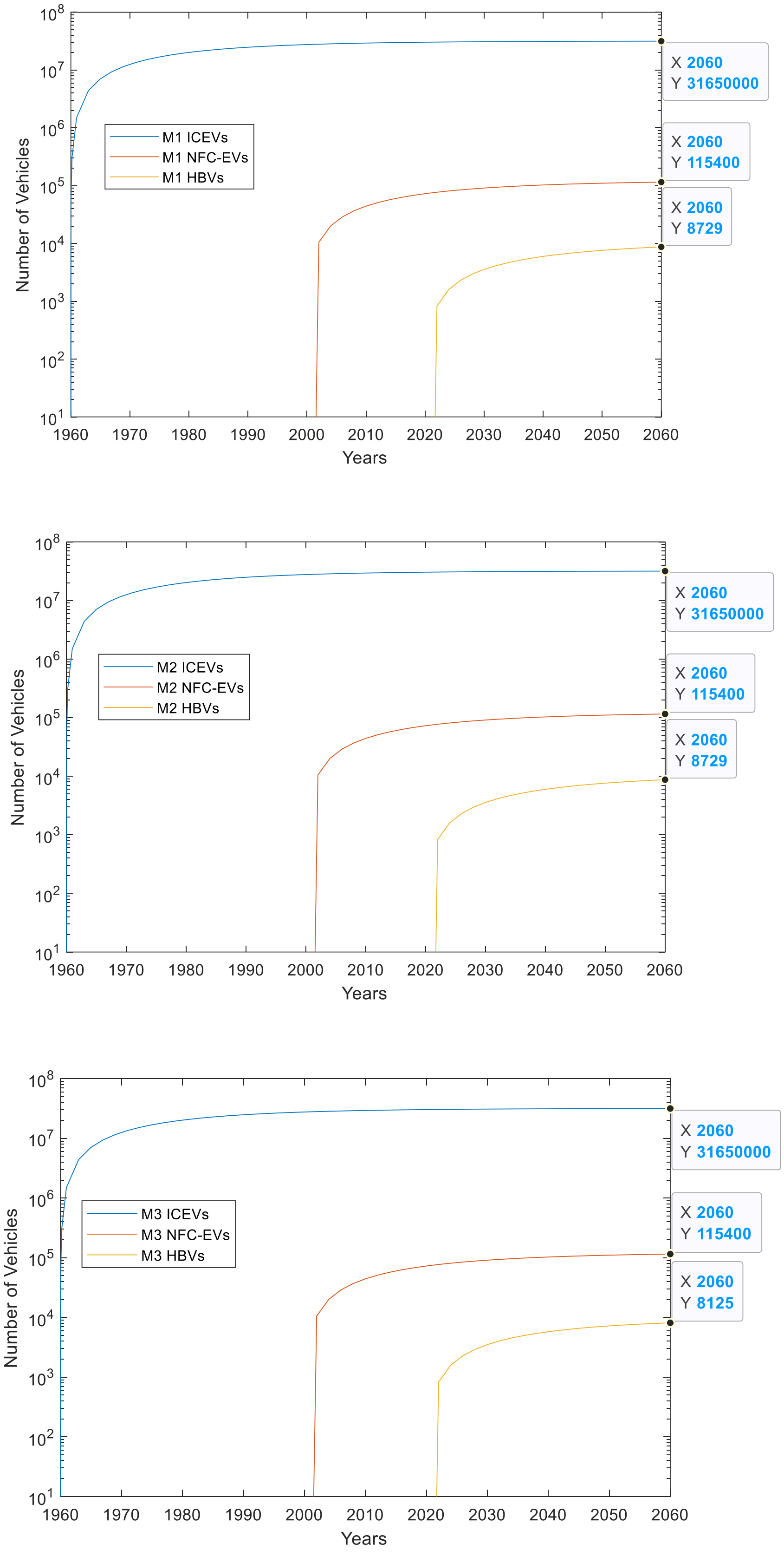


Figure 6. 7: Scenario 1 depicting the extreme penetration scenario for both NFC-EVs, and HBVs using M1, M2, and M3 models in order.

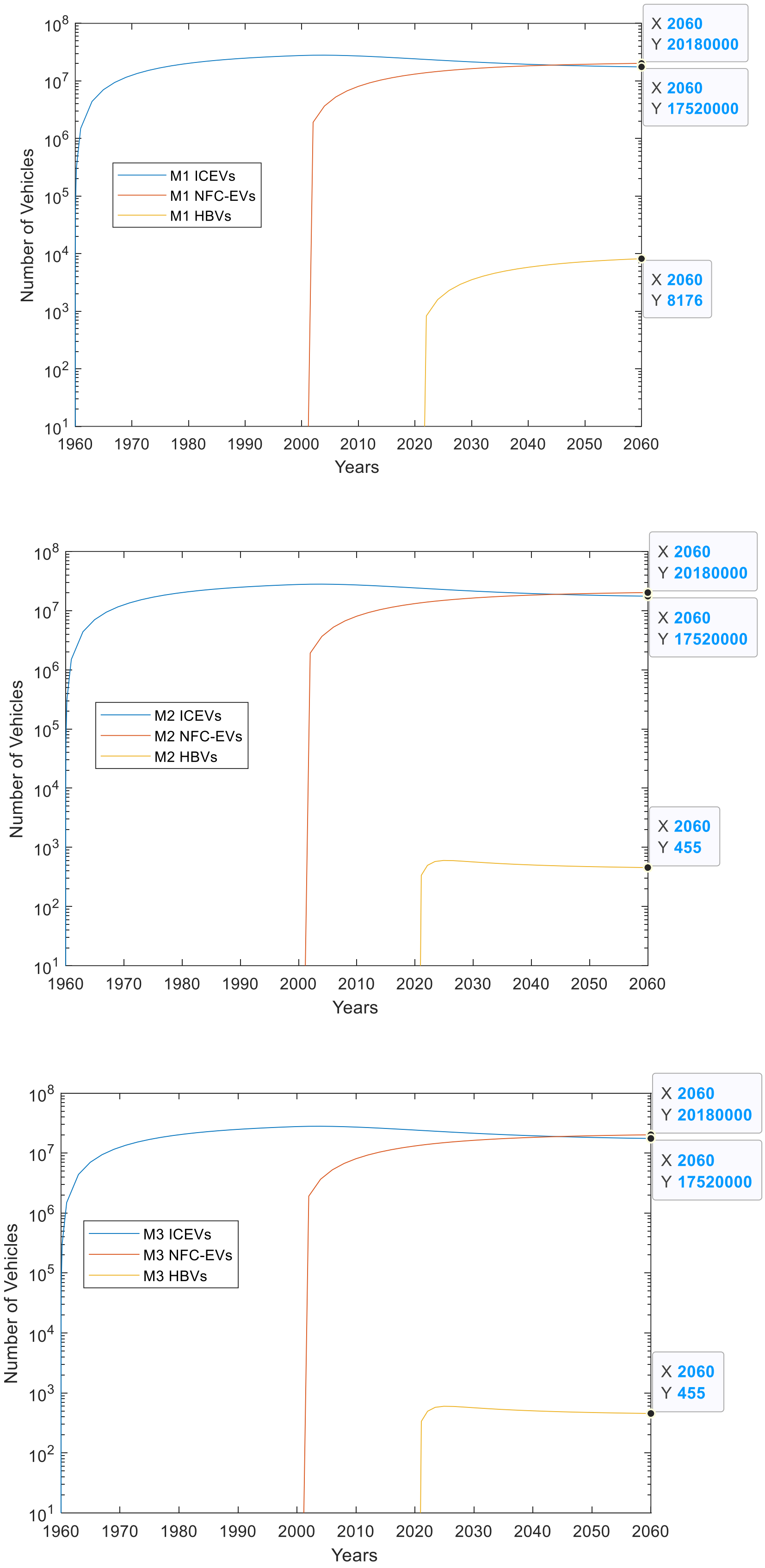


Figure 6. 8: Scenario 2: Moderate penetration strategy for NFC-EVs, and an extreme penetration strategy for HBVs using M1, M2, and M3 models.

Since fossil fuels are finite and conventional vehicles must be replaced, many researchers have attributed a larger market share for hydrogen (Rahmouni et al., 2016; Seo et al., 2020) than that indicated in scenario 1, which can be ruled out. Figures 6.8 shows fleet as depicted by the second scenario. The number of NFC-EVs increases to 17.62 million, while the number of HBVs remains negligible. This is a probable scenario, as currently, BEVs are becoming more widely available, and all the major vehicle manufacturers offer a hybrid/EV choice. In March 2020, 23000 mild hybrids electric vehicles were sold despite the pandemic (Wagner, 2020), suggesting that they are becoming increasingly popular. Here, it is assumed that NFC-EVs will continue and become the dominant vehicle types displacing a third of conventional vehicles. The remainder of conventional vehicles will be removed at the end of their lifecycle. EVs have the advantage of being charged at home, which eases the transition in terms of investing in a new infrastructure. Thus, in this scenario, stakeholders and the government have chosen to focus on NFC-EVs.

In terms of policies and investment, all three models behave in a similar manner, as in the case with scenario 1. The number of conventional vehicles drop from 30 million to 17.52 million under the constraints of the model as expected. In terms of HBVs, when the two predators are allowed to interact in the M2, and M3 models, the number of HBVs are further reduced. This is expected because NFC-EVs currently have a greater market share than HBVs, and a more readily available electrical refuelling infrastructure with the option of fuelling at home. Since NFC-EVs, receive the bulk of the funding and investment by deploying moderate strategy, when allowed to attack HBVs on an extreme penetrative strategy, reduced the number of HBVs. Thus, highlighting the strength and importance of policies and the role of the government.

The third scenario shows the scenario opposite to scenario 2 where in this case HBVs employ the moderate penetration strategy and NFC-EVs employ the extreme strategy (see figure 6.10). This is an unlikely scenario since hydrogen is competing against alternative vehicles such as EVs/hybrids as well as conventional vehicles. Since greater investment and stringer policies are required for HFCVs to attain a larger market share in the private vehicles sector in comparison to NFC-EVs, it can be concluded that they will have a stronger attack rate, thus penetration rate than HFCVs. Besides, hybrids/EVs have sold more vehicles than HFCVs as shown above and continue to be sold (Wagner, 2020). The models show that if resources and

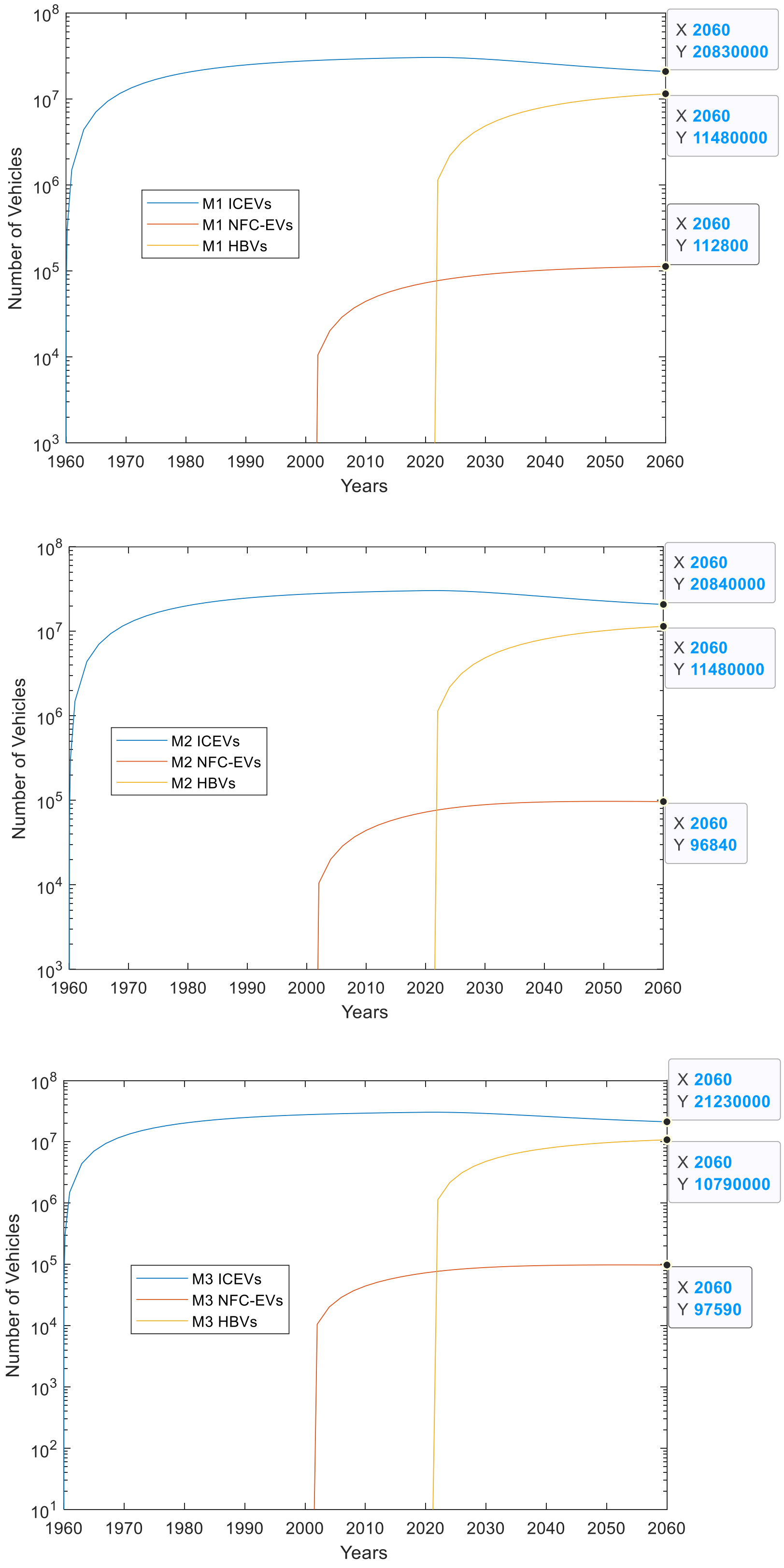


Figure 6. 9: Scenario 3 - Moderate penetration strategy for HBVs and an extreme penetration strategy for NFC-EVs using M1, M2, and M3 models.

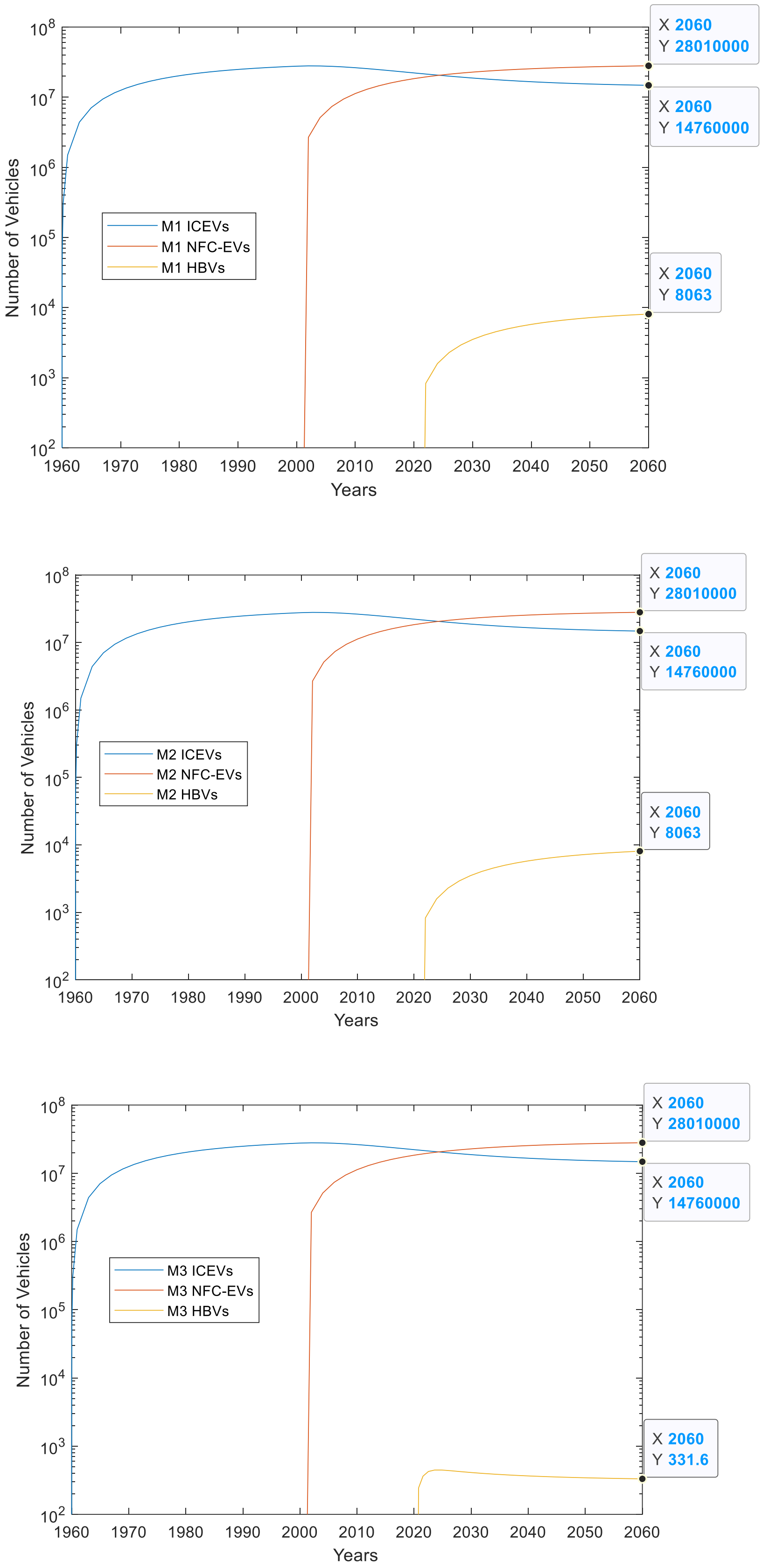


Figure 6. 10: Scenario 4 – Best penetration strategy used for NFC-EVs and extreme penetration strategy for HBVs using M1, M2 and M3 models

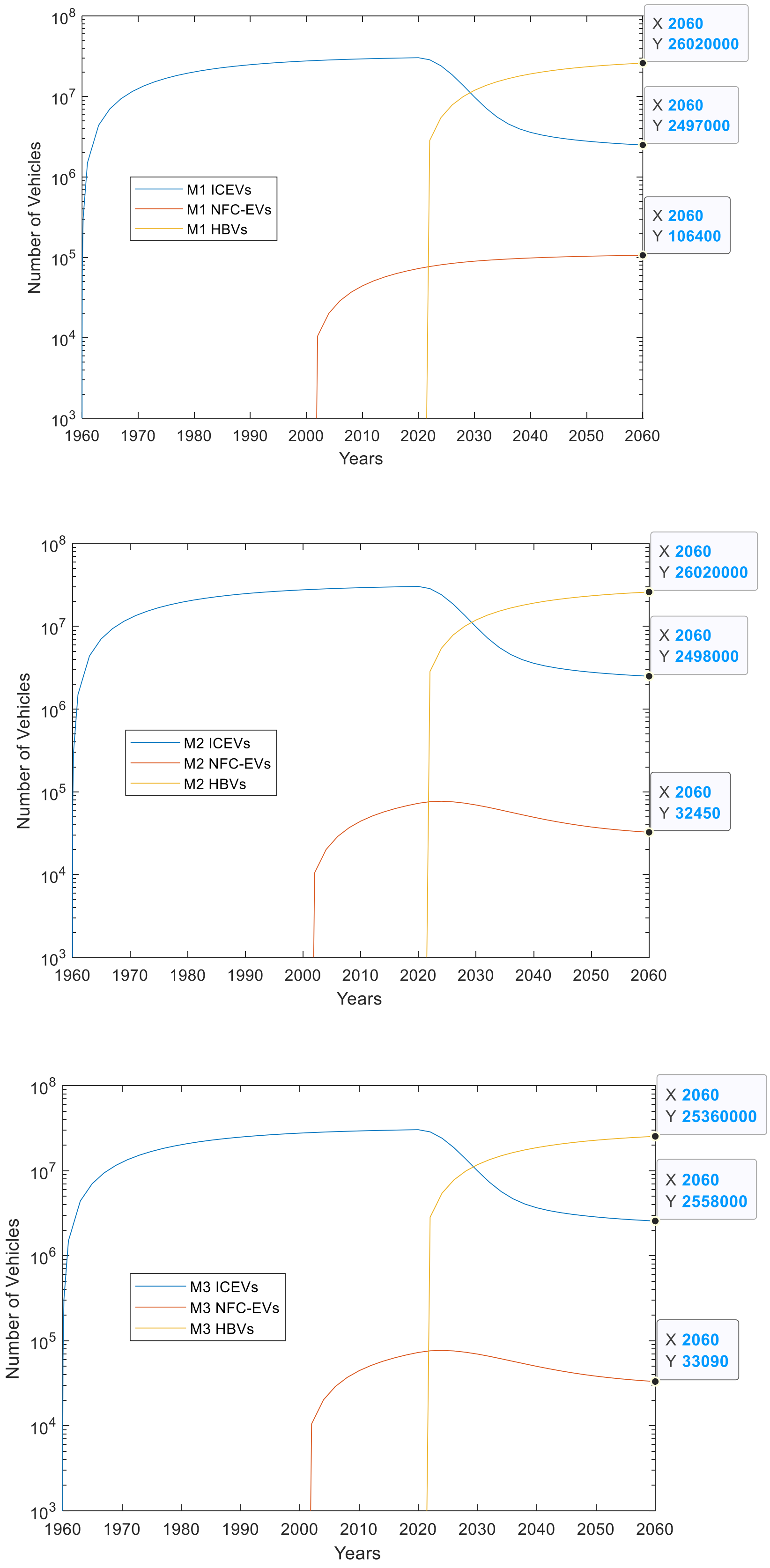


Figure 6. 11: Scenario 5 - Best penetration strategy used for HBVs and extreme penetration strategy for NFC-EVs using M1, M2, and M3 models.

investment are solely focused on a hydrogen infrastructure, then HBVs can reach a significant proportion of the market in expense to NFC-EVs.

In scenarios 4 and 5, NFC-EVs and HBVs each employ the best and extreme penetration scenarios alternatively. Currently, policies employed by the UK are favourable towards NFC-EVs to reach most of the market share as indicated in scenario 4 (see figures 6.11); for scenario 5 again is unlikely considering the private fleet alone (Figures 6.12). However if other energy sectors adopt hydrogen, then HFCVs can become dominant. McDowall (2014) also suggested that the role of hydrogen outside transport may be valuable as renewable energy is gaining market shares, which can help to facilitate the required infrastructure.

Figures 6.13 highlight that a strong strategy for NFC-EVs will really drive HBVs out of the market to current levels. The number of conventional vehicles dropped and then plateaued around 14 million. The fuel input of conventional vehicles remained the same throughout the simulations, and so only the direct impact of NFC-EVs and HBVs is demonstrated on the number of conventional vehicles. In reality, conventional vehicles will be penalised by clean air zones (BCC, 2021) and other initiatives, so the number of conventional vehicles will reduce first through penalisation before mass adoption of alternative vehicles. This is driven by the need to reduce emissions and meet environmental targets outlines in the policies by the government. Political sensitive issues affecting supply chains will also contribute immensely such as war, or a pandemic.

Scenario 5 (Figure 6.12 and table A.1) interestingly highlights that the best-case scenario for HBVs has negligible impact in the M1 model where both NFC-EVS and HBVs attack conventional vehicles only. Both NFC-EVs and HBVs follow their own trajectories based on the fuel input and parameters replacing conventional vehicles. The conversion rate of conventional vehicles into HBVs is lower than that of NFC-EVs on conventional due to current market proportion and infrastructure. Approximately 10 million more ICEVs were removed from the market based when NFC-EVs deployed the best-case strategy rather than HBVs. This suggests that for HBVs to impact in a similar manner, then more external help from policies and stakeholders is necessary.

Figure 6.13 further highlights that yet again when both NFC-Vs and HBVs can attack each other, the growth of HBVs is inhibited after an initial increase. This is expected because of the

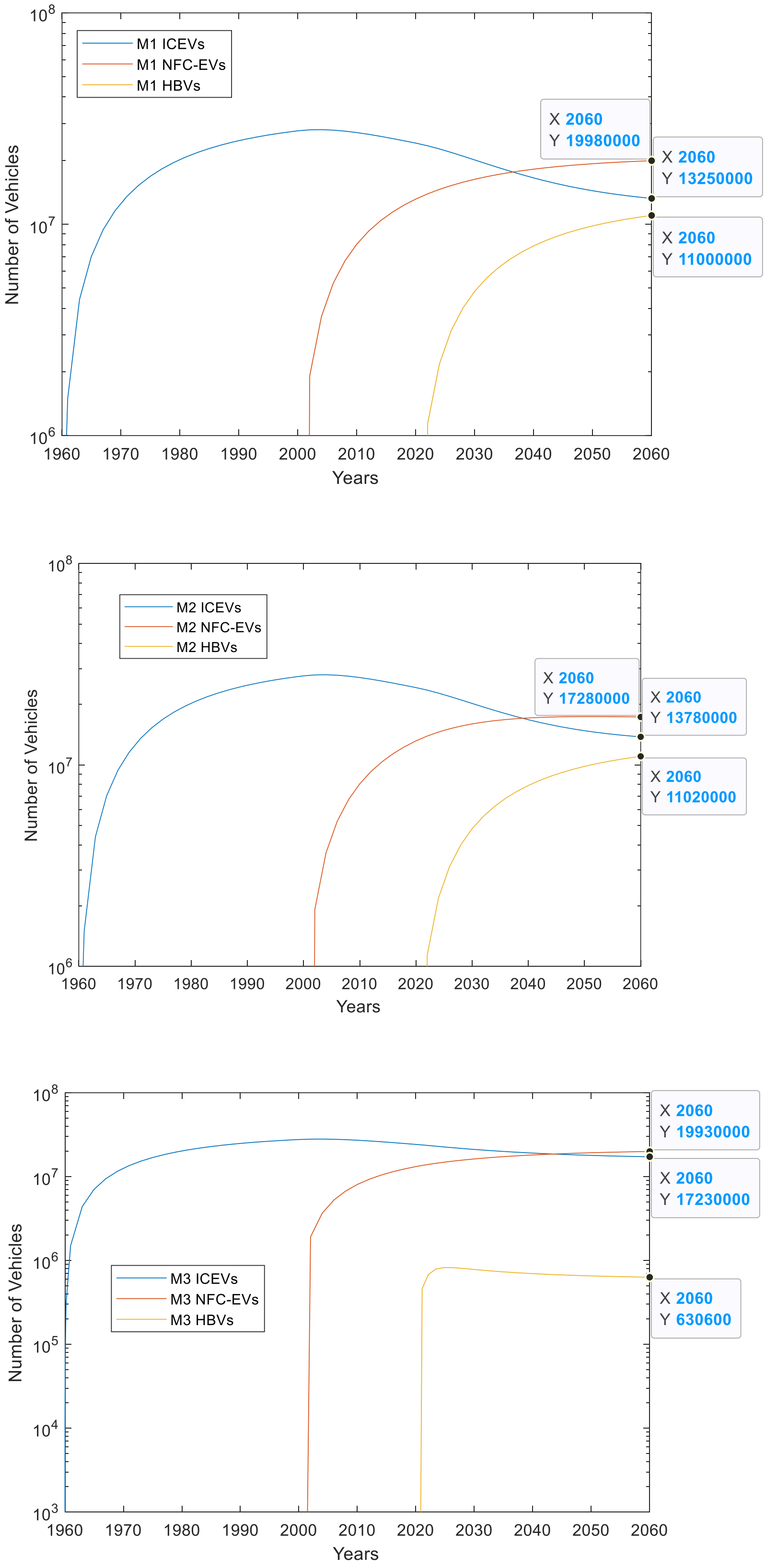


Figure 6. 12: Scenario 6 – Moderate penetration strategies employed for both NFC-EVs, and HBVs using M1, M2, and M3 model.

constraints on the model reflecting the given scenario and the current precedence of NFC-EVs over HBVs. New penalties on ICEVs, such as the introduction of clean air zones, can be shown by reducing the fuel input of ICEVs from 2020 onwards. This will incorporate the exaggerated drop in conventional vehicles that will drive the consumption of AFVs.

6.3.2 Strategies for the UK's outlook on the passenger vehicle sector

Current regulations and funding priorities suggest and demonstrate that NFC-EVs will form a greater proportion of passenger vehicles to replace conventional vehicles (HM Government, 2018; Netinform, a2019; UKH2Mobility, 2020). While HBVs are receiving more attention globally, the uptake of both HRS and HBVs is negligible, considering the entire passenger fleet and its refuelling infrastructure (GOV.UK, 2019). The market share of NFC-EVs is greater than HBVs of more than half a million vehicles and during the COVID-19 consumers still bought EVs and hybrids (Wagner, 2020). Since, the electrical infrastructure is established, and consumers have the option to charge at home, NFC-EVs have stronger outlook that HBVs, despite the benefits of HBVs over EVs. Many studies have also concluded that hydrogen will play a limited role for the private vehicle fleet (Talebian et al., 2019b; Seo et al., 2020; Yoon et al., 2022), this is clear in the scenarios proposed by the researchers.

Furthermore, as a baseline in this thesis, the infrastructure has been selected to operate at maximum capacity. However, this will not be the case. The hydrogen refuelling infrastructure will initially be under-utilised (H2ME, 2015) resulting in fewer HBVs on the road. This under-utilisation is captured by varying parameter h in the third-order models and manipulating the growth rate to reflect this. The input from government policies, current imbalance in investment corresponding to different technologies and the number of vehicles on the road is reflected by the endogenous parameters of the respected models.

The 3 prey – 2 predator third-order model is used in this section to assess various scenarios reflecting the UK's private vehicle fleet. The scenarios proposed consider both the current emphasis on hydrogen by governmental initiatives, number of hydrogen vehicles on the road, and the scenarios projected in the literature as mentioned above. Tables 6.10 – 6.13 show the results obtained from the third-order model consisting of 3 prey - 2 predators with various market share scenarios. The maximum market share obtained by HBVs is 50% and minimum is 20%. To meet the demand in the market once conventional fuel is eliminated must be replaced by a range of fuels to diversify the supply. The benefits offered by hydrogen in an inter-connected network covering different energy sectors cannot be ignored in transport. However, simply having a network of HRSs, or a centralised network does not necessarily mean that the uptake of HBVs will occur with certainty. For this reason, each market share level is simulated over 4 scenarios where the utilisation level of HRSs is varied: 100%, 75%, 50, and 25%. This will capture realistic scenarios of the future, where various stakeholders will invest in limited infrastructure, but the uptake of HBVs to utilise the hydrogen available will lag. The amount of fuel saved by the reduction in the number of conventional vehicles is also provided alongside the corresponding $C0_2$. Decarbonising the private fleet will ensure that carbon emissions will also reduce.

Table 6. 7: The number of conventional vehicles displaced using the M3 model is shown with market share of 80:20 for NFC-EVs to HBVs.

Proportion (%)	RS utilisation (%)	Number of ICEVs displaced (X1)	Number of NFC-EVs (X2)	Number of HBVs (x3)	Fuel Saved (kg/year)	CO2 reduction (kg/year)
Non-FC hybrids + EVs: HBVs 80:20	100	15,279,910	24,932,462	274,967	2.25e10	6.89e10
	75	14,982,355	25,220,600	165,272	1.651e10	5.05e10
	50	14,672,445	25,516,540	55,808	1.651e10	5.05e10
	25	14,591,966	25,594,056	27,871	1.651e10	5.05e10

0.75kg of petrol emits 2.3kg of C02; 0.85kg of emits 2.6kg of C02; Petrol and diesel are used in 50:50 ratio to determine the C02 reduced.

Table 6.10 displays the extreme scenario for hydrogen where only 20% of the private fleet market is captured. However, despite the infrastructure being in place the number of HBVs will lag and the Hydrogen infrastructure will be under-utilised initially. Therefore 4 scenarios for HBVs are depicted in the table. For NFC-EVs it is assumed the electrical infrastructure is utilised at maximum. When HRSs are operating at 100%, just over 2710 000 HBVs are supported by the infrastructure. The number of HBVs reduces to 27, 871 when the HRSs operate at 25%.

Table 6. 8: The number of conventional vehicles displaced using the 3 prey – 2 predator model with market share of 70:30 for NFC + EVs to HBVs.

Proportion (%)	RS utilisation (%)	Number of ICEVs displaced (X1)	Number of NFC-EVs (X2)	Number of HBVs (x3)	Fuel Saved (kg/year)	CO2 reduction (kg/year)
Non-FC hybrids + EVs: HBVs 70:30	100	15,176,604	21,330,342	567601	2.508e10	7.67e10
	75	14,511,661	21,799,023	338,541	1.542e10	4.72e10
	50	13,798,168	22,283,934	113641	1.541e10	4.72e10
	25	13,606,208	22,411,793	56,609	1.541e10	4.72e10

0.75kg of petrol emits 2.3kg of C02; 0.85kg of emits 2.6kg of C02; Petrol and diesel are used in 50:50 ratio to determine the C02 reduced.

Table 6.11 represents the second-least favourable scenario for HBVs, where only 30% of the market is captured. NFC-EVs represent 70% of the market. Despite the greater market share than the 80:20 scenario, at 100% utilisation, the HRS network only supports 567,601 HBVs. At 25% utilisation, the HRS network supports 56,609 HBVs.

Table 6. 9: The number of conventional vehicles displaced using the 3 prey – 2 predator model with market share of 60:40 for NFC + EVs to HBVs.

Proportion (%)	**RS utilisation (%)**	**Number of ICEVs displaced (X1)**	**Number of NFC-EVs (X2)**	**Number of HBVs (x3)**	**Fuel Saved (kg/year)**	**CO2 reduction (kg/year)**
Non-FC hybrids + EVs: HBVs 60:40	100	14,787,292	18,028,671	749,921	2.601e10	7.96e10
	75	13,816,821	18,553,679	445,475	1.418e10	4.34e10
	50	12,746,360	19,101,652	149,330	1.416e10	4.33e10
	25	12,451,184	19,247,979	74,256	1.416e10	4.33e10

0.75kg of petrol emits 2.3kg of C02; 0.85kg of emits 2.6kg of C02; Petrol and diesel are used in 50:50 ratio to determine the C02 reduced.

Table 6.12 represents the second-best scenario for hydrogen where 60:40 market share is attained in favour NFC-EVs. Just under 750,000 HBVs are supported by the HRS network when operating at 100% efficiency. The number of vehicles drops to 74, 256 HBVs when the network operates at 25% of the available capacity.

Table 6. 10: The number of conventional vehicles displaced using the 3 prey – 2 predator model with market share of 50:50 for NFC + EVs to HBVs.

Proportion (%)	**RS utilisation (%)**	**Number of ICEVs displaced (X1)**	**Number of NFC-EVs (X2)**	**Number of HBVs (x3)**	**Fuel Saved (kg/year)**	**CO2 reduction (kg/year)**
Non-FC hybrids + EVs: HBVs 50:50	100	15,065,922	14,535,226	1,147,972	2.751e10	8.42e10
	75	12,757,109	16023,856	643,978	1.276e10	3.90e10
	50	12,711,690	16,160,433	222,049	1.271e10	3.89e10
	25	12,700,363	16,217,464	110,901	1.270e10	3.89e10

0.75kg of petrol emits 2.3kg of C02; 0.85kg of emits 2.6kg of C02; Petrol and diesel are used in 50:50 ratio to determine the C02 reduced.

Table 6.13 represents the best-case scenario for HBVs where a market share of 50:50 is achieved with NFC-EVs. The number of HBVs supported by the HRS network when operating at maximum capacity is 1,147,982, and this reduces to 110,901 when the HRS is operating at 25% capacity. This is significant as it demonstrates an intent of purpose from all the stakeholders, however the number of HBVs on the road compared to NFC-EVs is significantly less. So, despite the funding and infrastructure in place, the uptake of NFC-EVs is popular and more favourable. At the point of under-utilisation, the loss in investment for stakeholders becomes greater. This suggests that investing in NFC-EVs is a stronger strategy for the UK moving forward.

Depending on the market share, the maximum number of conventional vehicles displaced due to the attack ates of NFC-EVs, and HBVs are approximately 15 million and the least just under 12.5 million. It is interesting to note that while the number of conventional vehicles displaced decreases as the HRS moves from 100% utilisation to 25% utilisation as expected. Furthermore, the number of conventional vehicles displaced decreases as the market share of HBVs increases. The number of conventional vehicles displaced by 50:50 market share is higher than market share 60:40. This is because the attack rate of HBVs increases as the market share of HBVs increases. Whereas, for the 60:40 market share scenario, the attack rate of NFC-EVs is reduced to reflect the market share and the attack rate of HBVs is also less aggressive.

Figure 6.14 depicts the market share between NFC-EVs and HBVs where the HRSs are operating at maximum capacity. It is interesting to note that the growth of HBVs is inhibited regardless of the market share when NFC-EVs can compete against HBVs. This represents the current state of AFVs, where majority of government funding is applied to hybrids and EVs with small investments allocated to hydrogen technology. This demonstrates that regardless of the market share attained by HBVs, HBVs will struggle to gain momentum when AFVs are also competing. Here, the Simulink graphs are given representing the case where the HRSs are utilised at 100% efficiency. Even under 50:50 of market share, just over 1 million HBVs were available in comparison to almost 15 million NFC-EVs. In comparison to the entire fleet the number of HBVs attained by the market share of 50:50 at 100% utilisation is less than 0.5%. So therefore, to reduce the under-utilisation period of the HRS, and placing resources at the more effective strategy of NFC-EVs, the 80:20 market share is the most sensible option for the UK.

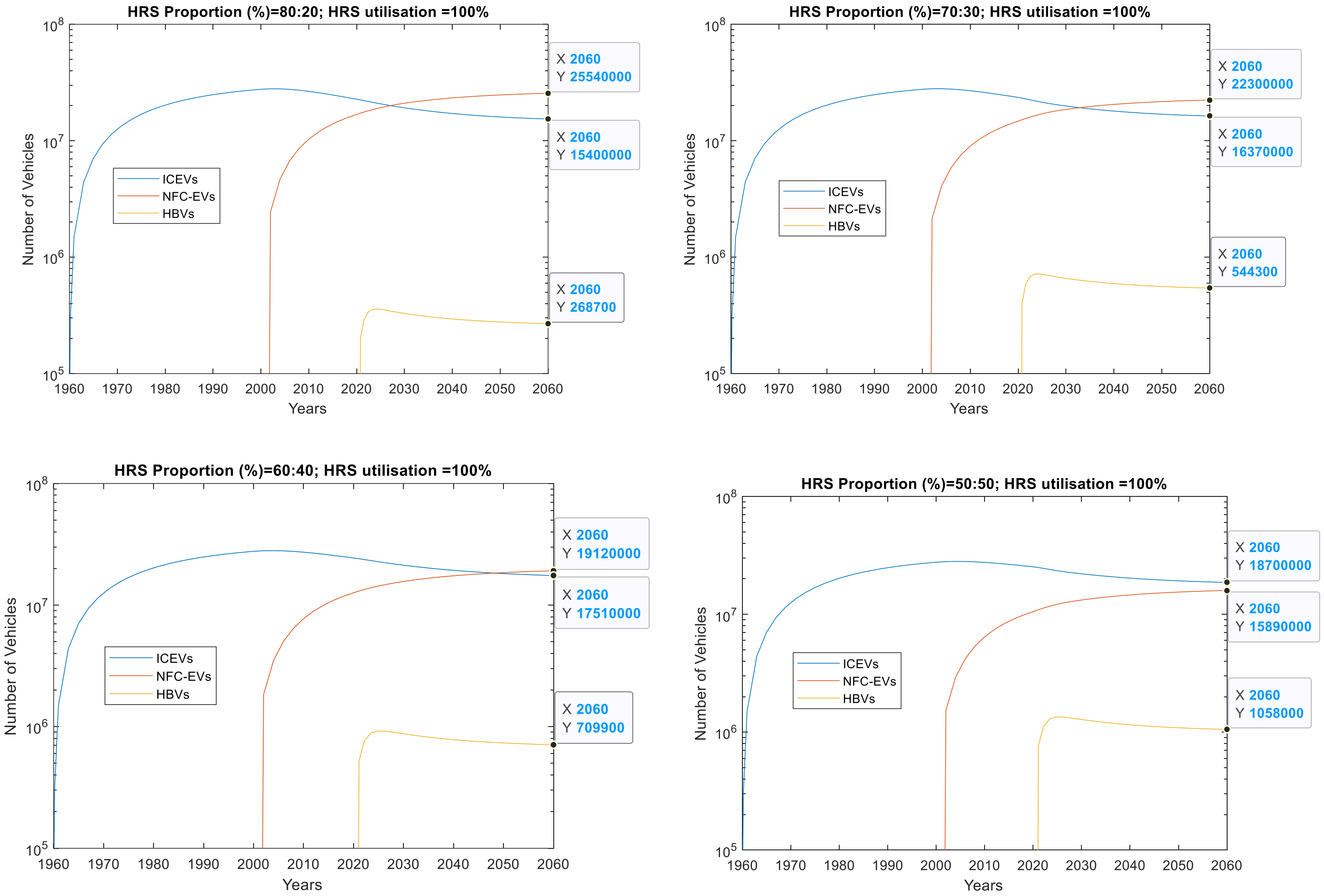


Figure 6. 13: The market proportion of NFC-EVs and HBVs at 100% efficiency

The 80:20 market share for HBVs was optimised using LQR to assess the stability of the system. Figure 6.15 represents the linearised model in terms of the number of vehicles over the next 50 years.

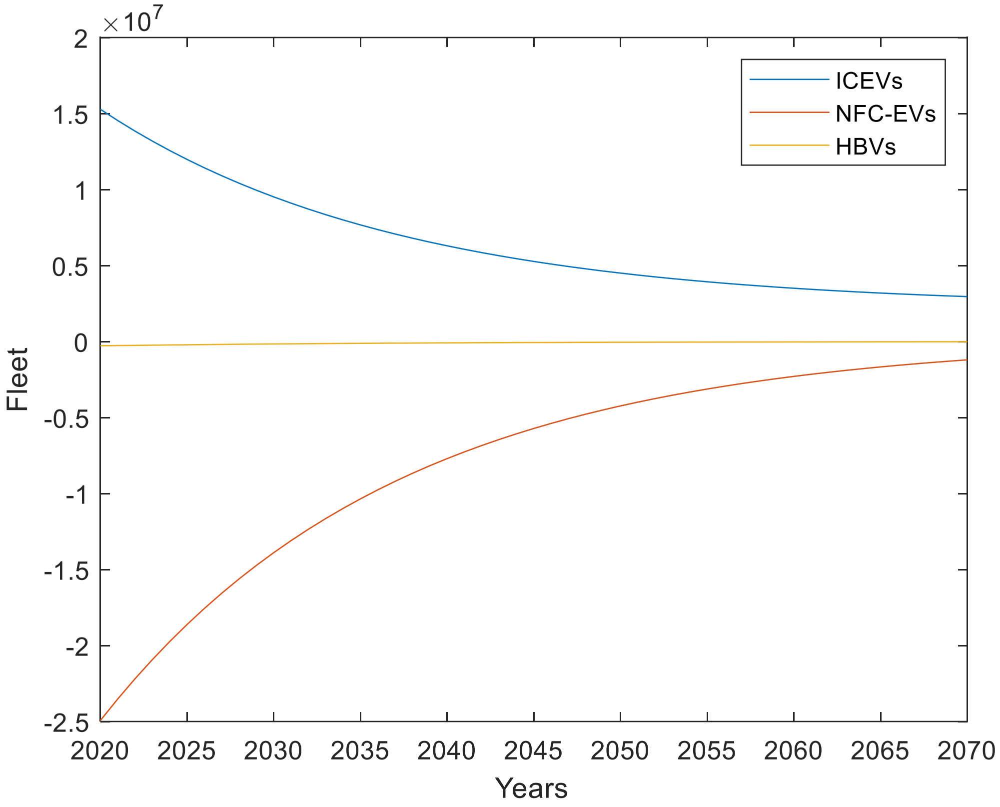


Figure 6. 14: Represents the linearised graph of the third order model

From previous results, hydrogen will be effective if a market share of 20% is achieved. However, the effectiveness of this depends on how soon the infrastructure is implemented eliminating conventional vehicles from the market, forcing consumers to make more sustainable choices. It is unlikely that alternative technology will be able to displace conventional vehicles on its own. This is evident because the UK has fallen short of meeting targets outlined by the government and other stakeholders (UKH2Mobility, 2020). External factors on the source and supply chains of crude oil through war, or diseases like the COVID-19 pandemic will compel governments to re-think strategies to alleviate the UK’s dependency on crude oil. Too often, the option of retaining consistency and keeping disruption to minimal is chosen. For these reasons, it is proposed that the decarbonisation of the UK’s private vehicle fleet has two options or strategies available. The first option is centred around the government who will sanction carbon emitting companies to reduce their carbon footprint, increases tax on fossil-based fuels and provide subsidies for alternatives. Political sensitivities affecting the supply of oil will also intensify the urgency to implement alternative provision. The second option is to keep disruption to minimal and prolong the use of oil for as long as possible whilst introducing alternative fuels over a period of 30 years. In the short-term, improving vehicle efficiencies and promoting better services for public transport. LQR is used to penalise conventional fuel, and the ICE of NFC-EVs to assess the effectiveness of the controller.

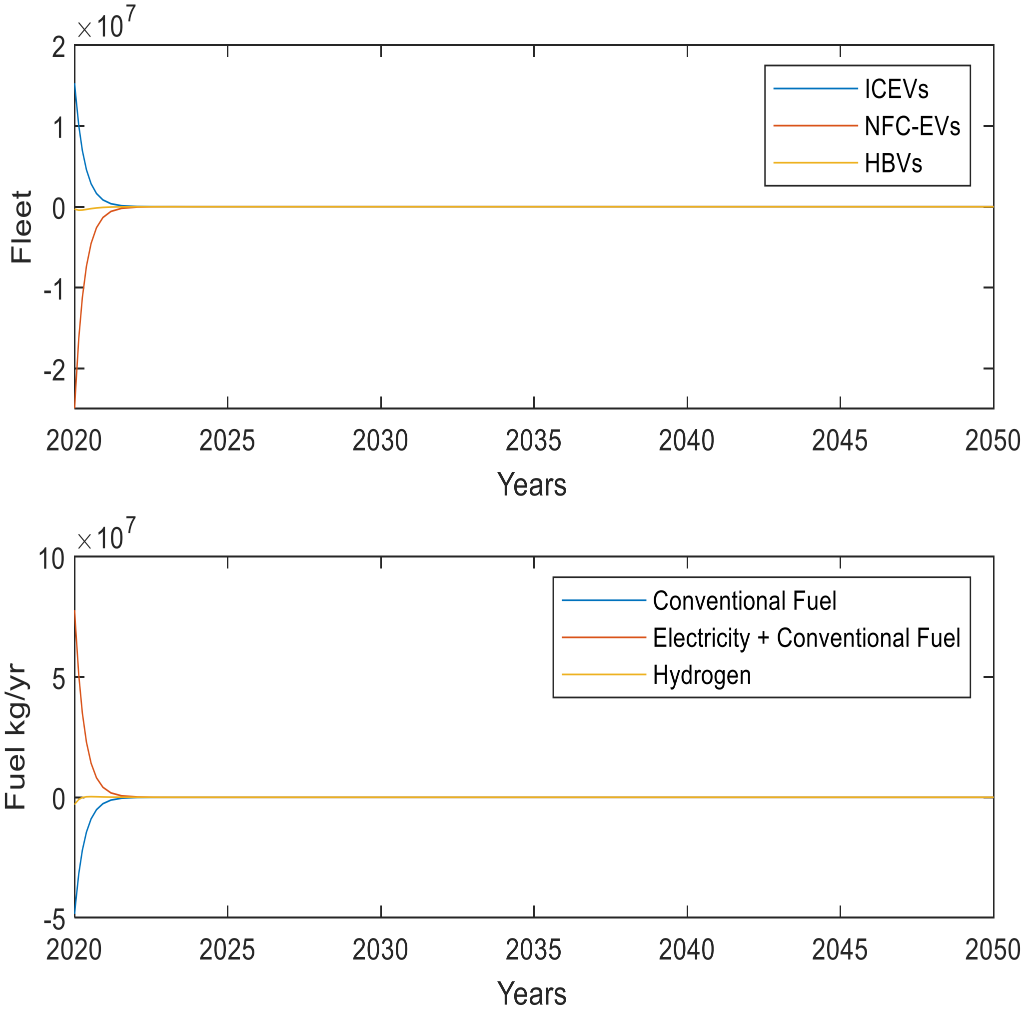


Figure 6. 15: Aggressive controller employed penalising the time taken to meet decarbonisation targets.

Considering the first option for the UK, the strategy envisioned is to decarbonise the UK within the next five years, exceeding expectations. Figure 6.15 represents this case. The states return to zero as soon as possible. This is the optimal solution but comes with a huge cost. An aggressive controller is deployed where the control is cheap i.e. irrelevant, and non-zero states are expensive. The importance here is associated with stopping all dependence on oil, thus decarbonising the private vehicle fleet ahead of targets. The control matrix, K, in this case, is very aggressive. The controller drives the number of conventional vehicles to zero quickly, and the uptake of alternatives.

Figure 6.16 depicts the second strategy for the UK where decarbonisation is spread across 30 years to ensure disruption to drivers, supply chains and all the stakeholders is kept to minimal. This will keep costs down by delaying or spreading the cost of building infrastructure for alternative fuels. In this case, the R value was given a higher value than Q, so that the states converged to zero slowly resulting in a conservative controller. The control is expensive in this case and the non-zero state is cheap.

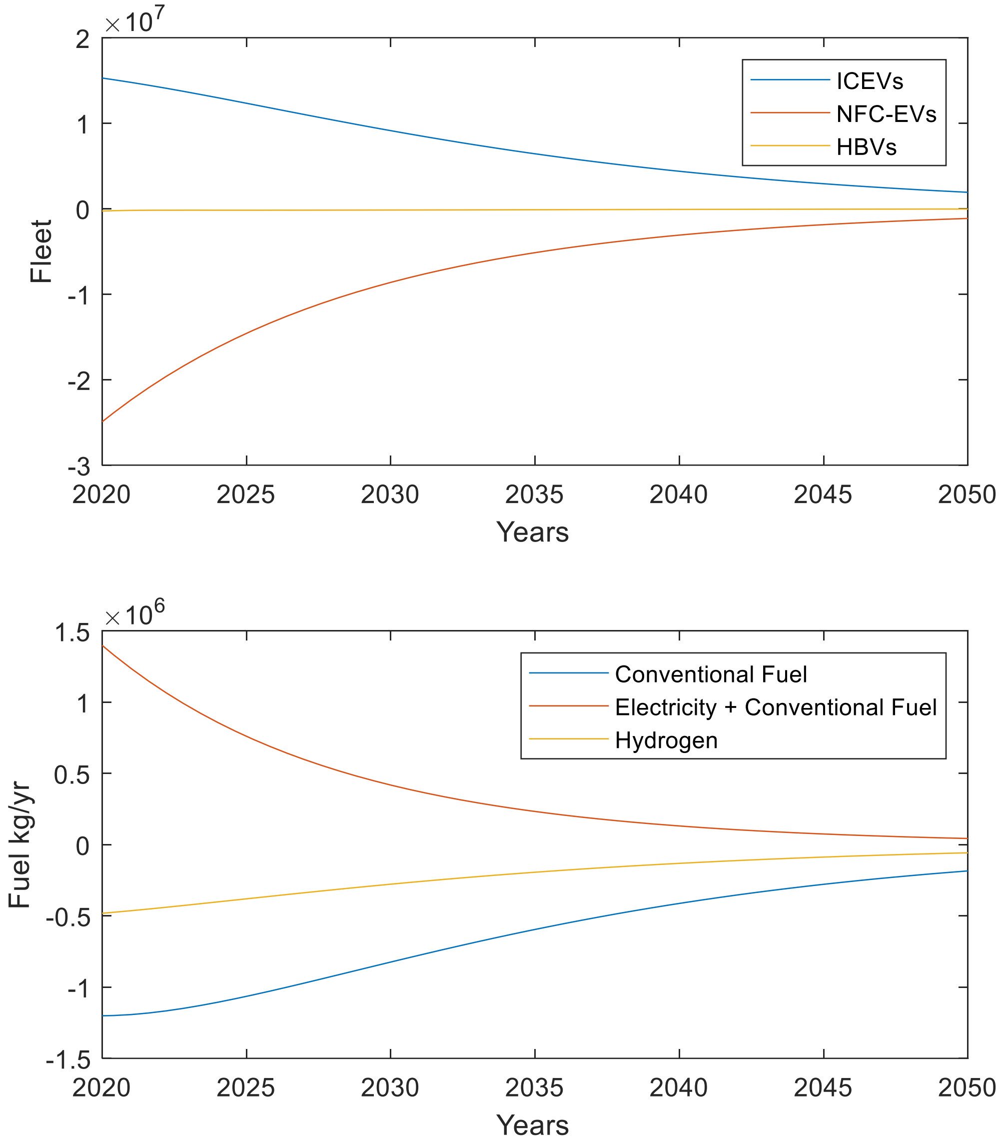


Figure 6. 16: Conservative controller deployed to minimise the disruption whilst decarbonising the private vehicle fleet.

To decarbonise the UK's private vehicle fleet, conventional vehicles must be penalised more than NFC-EVs. Attacking the ICE aspect of NFC-EVs. The UK must strive to eliminate its reliance on oil to decarbonise the private vehicle fleet, in addition to reducing disruption to drivers. Increased taxes, expanding public transport services, and investing in diverse alternative fuels will help to make the transition easier. Figure 6.17 presents variable controller that aggressively impacts conventional vehicles, moderately aggressive to NFC-EVs and conservative to HBVs. The sooner conventional vehicles are removed from the road, space opens for AFVs, further research and development for AFVs. HBVs require huge investments and relevant infrastructure in place before HBVs are available for consumers, to therefore a conservative controller will extend the period for the hydrogen strategy to be realised in the UK.

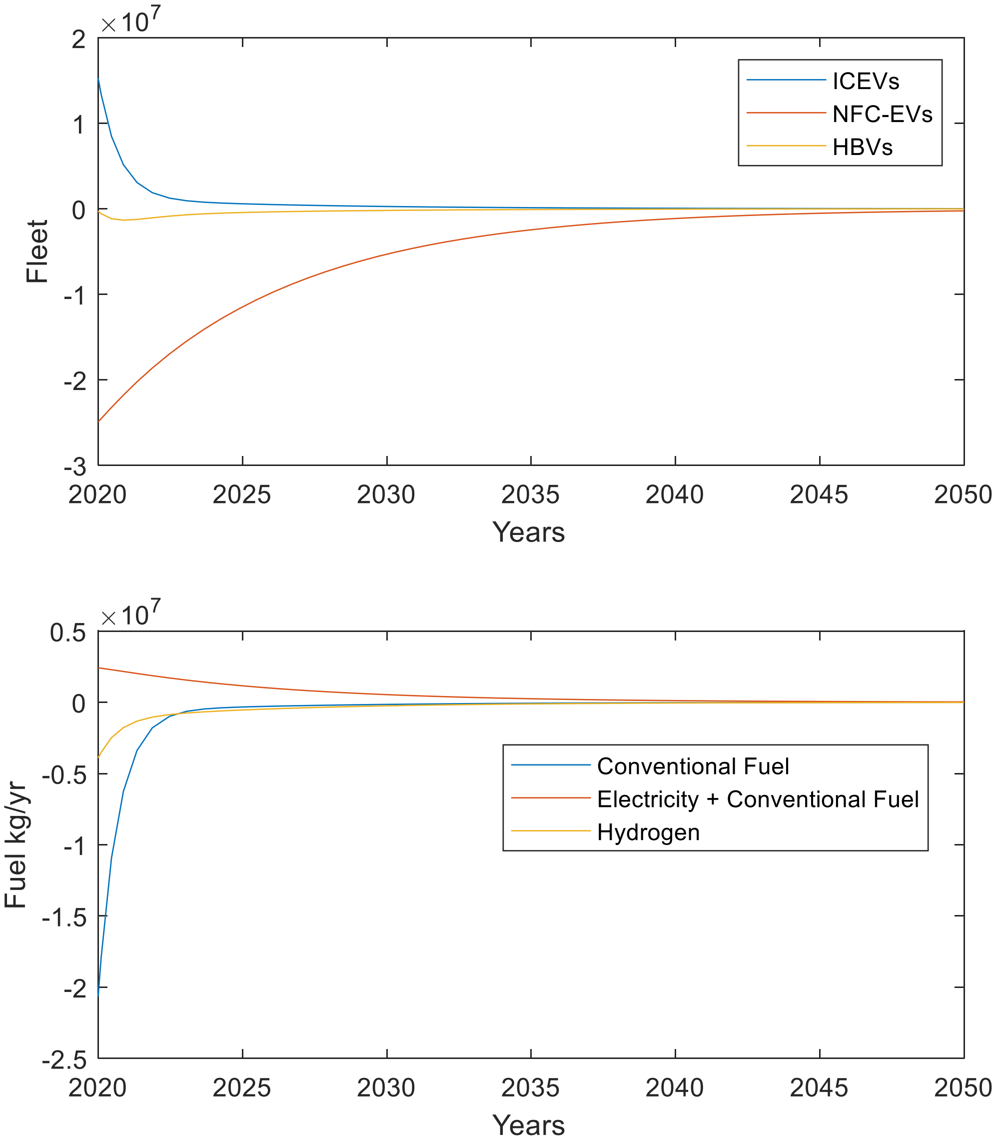


Figure 6. 17: Variable control

6.4 Discussion and Analysis

In response to the UK's need to transition from a fossil-based private vehicle fleet to a renewable energy-based one, this research focused on developing a dynamic model to explore the most effective strategies for the UK to deploy using LV and growth concepts. From the literature review, it was clear that the model must consider the impact of introducing new vehicle types on the current vehicle type, and the introduction and interaction of two or more vehicle types. For this reason, the LVM model was ideal as it considers the interaction between two or more technologies and the number of predators or technology being introduced can be increased to a multiple technology model. The LVM is associated with oscillating behaviour, which is useful for biological dynamic systems but not for the private vehicle fleet. To capture the growth of conventional vehicles and the subsequent decay once AFVs are introduced the growth model was developed in chapter 3. The first-order growth model was incorporated into the second-order LVM in chapter 4 with the case study presented in chapter 5. The third-order model developed in this chapter is the final development of the model presented in chapters 3, 4, and 5.

Some of the previous results are discussed in this chapter. The behaviour of the LVM was limited to reflect the growth of conventional vehicles in the UK. Once petroleum is replaced by alternative fuel it will not be introduced into the market because of limited supply and environmental impact. The growth model developed in chapter 3 was used to represent the growth of conventional vehicles in the UK realistically. Thus, the first-order model was used to modify the LVM to reduce the number of oscillations to reflect the private vehicle fleet. The LVM was chosen because of its ability to capture the interaction between two or more species/technology. Another benefit of the growth model was that it reduced the number of constraints and variables that alternative models considered to determine the hydrogen demand, such as household income and the number of vehicles per household. Other studies have considered the introduction of HBVs by considering SCs, however, in this case the growth model was used to consider the introduction of HBVs from a holistic viewpoint i.e., the entire private vehicle fleet.

The modified LVM was effective in simulating the growth of HFCVs, which corresponded to that obtained from the literature. The capacities of large HRS need to be increased to encompass a significant number of HFCVs into the private vehicle fleet, currently 100 HRES of 8064kg/day capacity each can only provide hydrogen for 1.12 million vehicles. When under-utilisation is considered, the number of HBVs drops even more making the prospect of using hydrogen as a fuel very unattractive. Furthermore, to bridge the gap between pre-commercialisation and an established market HFC-REs are expected to play a significant role. This also increases the capacity of the HR network capacity in that the number of vehicles supported sees an increase of 75% vehicles when half the vehicles introduced are range-extenders. Large centralise stations must be developed as soon as possible for sustainable growth in the sector regardless of the hydrogen demand for vehicles.

This chapter considered the introduction of hydrogen as a transportation fuel for passenger vehicles in the UK. The model proposed in chapter 4 was used to simulate different scenarios obtained from literature to evaluate the model developed against current SC proposals. From the results section, the model was able to simulate the different proposals across the timescale of 2020/2060, and if required, over the timescale proposed in the respected papers.

Three different proposals were selected covering a wide range of projections for the UK, such as conservative (UKH2Mobility, 2013), moderate (Moreno-Benito et al., 2017), and optimistic (Almansoori and Shah, 2012) projections. The UK's current level of investment is minimal in line with the UKH2Mobility report. If the investment for hydrogen follows this route, then hydrogen will not play a significant role in tomorrow's passenger vehicle fleet. The UK's current progress is near the most extreme scenarios proposed by Almansoori and Shah as well as Moreno-Benito et al. The UkH2Mobility report expects a sizeable infrastructure in place by 2030, which can support 1.18 million (2.d.p) or 3.92 (2.d.p) million HFC-REs. This only covers 3.93% or 13.1% of the passenger vehicle fleet operating at maximum capacity.

This case study assumed that the upper limit for hydrogen is if the entire private fleet was replaced by HBVs, however current analysis suggests that conversion of half the private fleet is optimistic. Therefore, it is improbable that a complete transition to hydrogen will occur. Furthermore, the model investigated the role of hydrogen and conventional vehicles. However, several vehicle types are expected to compete with conventional such as EVs, and hybrids. The model proposed in chapter 4 is extended to a third order model to allow multiple AFVs to compete with conventional ones to overcome these limitations. Hydrogen penetration scenarios are also limited to 50% of the private vehicle fleet.

This thesis developed the third-order model to analyse the interaction between multiple vehicle types, as is the case in the private vehicle sector. However, different proposals can be considered in terms of how the different vehicle types compete in the sector based on policies, performance, convenience, and funding. Tables A.1, A.2 and A.3 show the simulation results of six scenarios using the three third-order models. The results are visually clustered in figures 6.7 – 6.12. Different scenarios were decided by manipulating the fuel input parameter. This was set according to the type of strategy each employed, e.g., extreme-case. Other studies have also derived the hydrogen demand in a comparable manner, such as the work of Johnson et al. (2008), who derived the hydrogen demand based on the fixed percentages of state-wide HFCV penetration. In other words, 10% of HFCVs was considered to represent 10% of the vehicle market. This highlights that considering the role of hydrogen alongside other alternative fuels is important to understand the dynamics of the future private vehicle market.

For all six scenarios, the third-order models behave in a similar manner except in the case of scenario 6, where both predators employ a moderate strategy. For both the M1, and M2 models, HBVs, and NFC-EVs saw moderate growths, where the market share is 16.8 and 11.8 million each, respectively. However, for the M3 model, enabling NFC-EVs to attack HBVs inhibited the growth of HBVs (figure 6.10). This is also noticeable in figure 6.8 where both HBVs and NFC-EVs supported extreme strategies. This suggests that having the same penetration strategy for the two predators where they can attack each other will inhibit the growth of the one with a weaker attacking rate. Current policies and investments suggest that hybrids and EVs are receiving majority of the funding from governments and so will have a stronger attack rate than hydrogen. Without increasing the investment into hydrogen dramatically the growth of hybrids and EVs will outstrip and hinder that of hydrogen. Currently, consumers prefer EVs to HBVs due to the differences in infrastructure and prices (Shin et al., 2019). The UK government should allocate a separate fiscal investment for implementing the HRS network, rather than a combined one for zero-emissions vehicles or ultra-low emissions vehicles. It is more likely that hydrogen will be utilised on a smaller scale for specialised cases such as a fleet of taxis or buses such as the hydrogen-powered buses proposed for Birmingham in April 2021 (Mavrokefalidis, 2020). The purpose of alternative fuel vehicles is to reduce the reliance on fossil fuel with the least disruption to the current system. Considering that battery technology has made improvements and other hybrid technology will improve, it is easier to focus on EVs and hybrids than setting up a new infrastructure on such a scale.

The results indicated that solely investing in either type of vehicle heavily while moderately with the other is not enough to displace all the vehicles. The number of conventional vehicles did not decline to zero in any case, and it is likely that specialist vehicles and/or vintage vehicles will still use conventional fuels. The governmental intervention will be necessary to reduce the emissions from the transport sector as most vehicles will be removed from the road at the end of their lifecycle or through a scrappage scheme. The initial drive to manufacture AFVs in mass production must be driven by the government and local authorities. This is seen by the introduction of schemes such as clean air zones where drivers are being penalised for driving older conventional vehicles that are not fuel economical. In addition to this, some borough councils in the UK have been designated as the ‘Air Quality Management areas’ to test vehicles at the roadside issuing fines to drivers whose vehicles do not comply with new emissions standards (Emissions testing, 2021). The New European Driving Cycle (NEDC) with the Worldwide harmonised Light vehicle Test Procedure (WLTP), and Real Driving Emissions (RDE) makes vehicle manufacturers more accountable (VCA, 2020).

Section 6.3.2 presented the results of selected scenarios that consider the penetration of hydrogen realistically under different HRS utilisation and market share. Unless hydrogen technology receives special grants and funding from the government, only specialist and certain models may prevail bearing in mind the renewable energy sources that hydrogen is made from is in direct competition with hydrogen too. Hydrogen biomass may be the route for hydrogen in the future, but this will not provide the solution for transport. Since NFC-EVs are in a stronger position than HFCVs, and less dependent on the establishment of a new HRS network, having a market share of 80:20 is ideal since vast majority of the passenger vehicles are replaced by NFC-EVs. The findings here are in line with those by De-León Almaraz et al. (2015a), who proposed that a market share of 25% will be attained by HFCVs. Besides, as the proportion of HFCVs is increased with respect to NFC-EVs, the number of HFCVs remain modest. However, the greater attack rate deployed by HFCVs reduces the number of conventional vehicles without being replaced equally. So, to keep the number of vehicles constant and reduce overall costs of implementing an infrastructure greater than need, it is recommended that the UK aims to establish a market of 80:20 in favour of NFC-EVs.

An interesting point to note from the results associated with the market share of 80:20 considering the HRSs operating efficiency, there is a 53.7% reduction in $C0_2$ emissions between 100% efficiency and 75%. There is a reduction of 0.26% $C0_2$ emissions between 75% and 50%. So, with respect to emissions, deploying the hydrogen infrastructure at 20% market share, where potentially the HRSs are operating at 75% efficiency, will effectively reduce the under-utilisation period, allowing the station to meet up to maximum capacity at times reducing further $C0_2$ emissions while keeping the infrastructure minimal. Talebian et al. (2019) also found that the benefits in emissions reduction outweighed the additional costs by a factor of 4 at the pessimistic scenario. For, moderate and best-case scenarios, the infrastructure is both environmentally and economically competitive. In our case, the impact of NFC-EVs was considered alongside HBVs. As the proportion of HBVs increased, the proportion of NFC-EVs decreased. So, therefore the rate of ICEV's decay slowed down because NFC-EVs have a greater weighting than HBVs.

Furthermore, the quantity of hydrogen required to sustain 6 million vehicles at 20% of the market share will require considerable investment into the infrastructure. Considering HFCVs only, $1.56e^9 H_2/kg$ of hydrogen is required, considering HBVs combined at a ratio of 50:50, then $1.014e^9 H_2/kg$ is required, and considering HFC-REs only, then $4.68e^8 H_2/kg$ of hydrogen is required. One of the limitations of the work is that the hydrogen aspect of HFC-REs is considered only, and not the electrical aspect. So, in this case, further investment into the electrical infrastructure is also required to meet the additional demand. Since large HRSs have the capacity of $1000 H_2/day$, 4273 HRSs must be built to sustain demand for 6 million HFCVs at 100% operating efficiency. Furthermore, 5699 HRSs will be required which largely operate at 75% efficiency. According to the report by National Renewable Energy Laboratory on hydrogen station cost estimates (Melaina and Penev, 2013), the cost of a larger station of capacity 1500kg/day, operating at 80% has a total capital cost of $5.05M and a capital cost per capacity of $3370 per kg/day. This suggests that the ideal method to deploy to achieve the required hydrogen quantity is by investing in a large, centralised infrastructure, where excess hydrogen can be utilised in other energy sectors. This is in agreement with literature where a centralised network is preferred when the hydrogen demand meets a significant proportion of the market sector, for instance, some studies have (Seo et al., 2020; Agnolucci et al., 2013) suggested that centralised network and storage systems become important when HFCVs obtain a market share between 15-30%.

Figure 6.14 shows the linearised and figures 6.15-17 shows the optimised Simulink graph using LQR. The aim here was to increase the decay rate of conventional vehicles to speed up decarbonisation of UK's roads. The market share of the optimisation was selected as the 890:20 market share in favour for NFC-EVs. This is achieved by using an aggressive controller, K, so that the states return to zero as soon as possible. This is a scenario that is possible through SC disruptions or sanctions on the countries that provide oil. Finding alternatives and pushing the agenda of conserving the environment will facilitate the UK to achieve its targets of decarbonisation within 5 to 10 years. In addition to increasing the growth of AFVS. In this case, the deployment of 20% market share of HBVs is considered. The second option for the UK is to use a conservative controller to maintain the current set-up for as long as possible, with minimum disruption to drivers and achieve decarbonisation around 2050 in line with current targets. Disruptions to SCs, increase in fuel costs influences consumers to make behavioural changes and stakeholders to diversify fuel stock. For these reasons, using a variable controller that aggressively penalises conventional vehicles to set the agenda, whilst conservatively penalising AFVs will help to transition to make the transition from a fossil-based fleet. This will create the need to replace conventional fuel and give manufacturers time to manufacture and deliver AFVs to meet the demand, and stakeholders and government to ensure sufficient infrastructure is in place. This study considers the perfect-foresight formulation in that it optimises over the full-time horizon. In the real world, decision makers do not act with perfect foresight i.e., with uncertainty, making risky investments requires compensation for the risk resulting in higher cost.

While this research proposes promising results, the following limitations must also be considered.

1) Assumptions were necessary to consider in the research to simplify the modelling. However, further research can consider these to assess the impact on the modelling behaviour.
2) The attack rate of the NFC-REs and HBVs were determined by considering policies, environmental legislation, current fiscal pledges, vehicle sales, and infrastructure sales. So therefore, to translate the impact of these into account arbitrary values were allocated for the attack rate. So, for instance, 1 NFC-EV will replace 1 ICEV in all three penetration strategies. 0.5 a ICEV will replaced by a HBV in the moderate penetration strategy.
3) Another limitation of the study is that both HFCVs and HFC-REs were combined in a ratio of 50:50 throughout chapter 6. Vehicle manufacturers may favour HFCVs or HFC-REs solely.
4) The electrical fuel source of HFC-REs was not factored into the model as the primary focus was on hydrogen and reducing the complexity of the modelling.

6.5 Conclusions

In this chapter, the third-order model was considered to analyse multiple vehicle types competing to displace conventional diesel and petrol vehicles. From the three variants propose, the M3 model reflects reality more suitable than the other two. This is largely due to current policies and that the various technologies under consideration are direct competitors with each other. The main conclusion from the chapter is that HBVs will not be the sole solution to reducing emissions from the private sector nor play a substantial role. HBVs most likely will play a niche role in the sector, perhaps replacing specialist vehicles like ambulances and taxis etc. Considerable independent funding is required for a substantial infrastructure to be built thus allowing HBVs to flourish. As suggested by Tlili et al, (2020), stakeholders in the private vehicle sector should work closely with those in others sectors to prevent under-utilisation of the HRS network. The best-case scenario for the UK is to focus primarily on NFC- EVs in a ratio of 80:20 to HBVs. Despite, the 20% market share for HFCVs, a centralised approach will be more cost-effective than localised, decentralised network. This will enable the replacement of conventional vehicles largely whilst being a cost-effective strategy. Conventional vehicles must be penalised disproportionally with respect to the ICEVs of NFC-EVs, to induce behavioural changes in consumers considering purchasing or retaining conventional vehicles. This will also create the market demand for AFVs, thus solving the chicken-egg problem for hydrogen and other alternative fuels.

The results of the third-order model are summarised as follows:

1) The three variants of the third-order model enabled multiple vehicle types to compete in the passenger vehicle market.
2) The difference in M1, M2, and M3 allowed some of the policies to be taken into consideration endogenously.
3) The M3 model is most suitable to represent the UK's passenger vehicle fleet, and LQR can be utilised to optimise the period of decarbonisation of the passenger fleet.
4) HBVs is recommended to attain a 20% market share due to balance cost, emissions, and resources consumed for large-scale infrastructure.
5) Centralised hydrogen is the ideal path for the UK, both in terms of infrastructure cost and the quantity of hydrogen produced.
6) 75% operating efficiency of HRSs is recommended increasing to maximum use when necessary to avoid under-utilisation.
7) Conventional vehicles must be penalised to drive the transition by creating the market need for manufacturers and stakeholders to meet.

Chapter 7: Conclusions and further work

7.1 Introduction

This chapter begins by presenting the summary of the objectives with an explanation of how they were achieved highlighting the main contributions made. The chapter concludes by making recommendations that can be used as a foundation for future research in the areas of dynamic modelling and control for introducing disruptive technology.

7.2 Conclusions

To summarise, this research proposed a dynamic model to explore the effective pathways or strategies for the UK's private vehicle to transition to a hydrogen-based one using LV and growth concepts. Four objectives were outlined to achieve the aim of the thesis. Objective one was achieved by conducting a literature review of hydrogen infrastructure proposals for road transportation. The hydrogen demand was analysed in depth assessing the factors considered to model the demand and their input into the refuelling infrastructure. The review identified gaps in the literature where limited number of studies have explored the UK's private fleet using a diverse range of models and hydrogen estimation methodologies. In addition, no previous study considered the impact of conventional vehicles on HFCVs, nor considered the private fleet holistically. The estimation of hydrogen, in previous studies is assumed from scenarios predicted. Limited data for the UK is available in terms of AFVs, and data for HFCVs is not yet available. So, therefore the need to use current data for conventional vehicles, the current growth of conventional vehicles becomes important assuming that the market will continue to grow in a similar manner.

The second objective looked to propose a dynamic model assessing the introduction of HBVs into the UK's vehicle market using different scenarios. The dynamic model was developed in iterative steps over chapters 3, 4, and 6 based on the LVM and growth concepts. The LVM can be considered as an effective tool in predicting the growth of a new vehicle type into any vehicle market. The introduction of HFCVs into the private fleet is difficult to model due to the lack of historical data and insights to forecast recent technology. AFVs are considered recent and have limited data available from the UK's official statistics, and the data for HBVs is unavailable. The first-order growth model developed in chapter 3 directly over comes this issue by modelling the growth of HFCVs over 50 years using the growth rate of conventional vehicles over the last 50 years. The growth rate is an important parameter as it has been shown to be influential on the model characteristics. It is important to consider the growth of the market before integrating it into the LVM, to limit the oscillatory behaviour of LVM to reflect the private vehicle fleet. This was limited to reflect the growth, and subsequently, the decay of conventional vehicles. This was important because conventional vehicles will not see a revival due to the limited supply of fossil fuel and its corresponding environmental impact, see chapter 3.

The model was validated by simulating the HRSs at 100% to determine the hydrogen demand. The current literature has largely ignored the impact of HFCVs on conventional vehicles, and the push-back from conventional vehicles through the availability of feedstock and established supply chains, and refuelling infrastructure. This element of interaction between the vehicle types was captured by utilising the LVM to represent the introduction of HFCVs into the current vehicle market. The results were then compared to those worked out from the literature to assess the parameters selected and if the model was suitable. Furthermore, the results from chapter 4 indicate that it is possible to predict the growth of new technologies introduced into the market inclusive of investment levels, policies and based on previous growths of similar technologies. So, therefore contributing to data and insights to generate realistic forecasts for introducing HFCVs into the private vehicle market as shown in chapter 4.

The third objective was to critically evaluate the model developed against current supply chain proposals and frameworks. The third objective was addressed in chapter 5 where different proposals from the literature forecasting the growth of hydrogen in the UK were simulated using the developed model. The results showed that many of the proposals were optimistic in terms of market penetration and share HBVs, and different methods were used to calculate the hydrogen demand. According to current legislation, funding, and investment, the hydrogen infrastructure is not sufficient to attain a significant market share, nor is it on the route to attaining it. If the investment for hydrogen follows this route, then hydrogen will not play a significant role in tomorrow's passenger vehicle fleet. The UK's current progress is near the most extreme scenarios proposed by Almansoori and Shah as well as Moreno-Benito et al. The UkH2Mobility report expects a sizeable infrastructure in place by 2030, which can support 1.18 million or 3.92 million HFC-REs. In any event, it is highly unlikely that HRS will operate at maximum capacity all the time, and so fewer HBVs are expected to be on the road as shown in chapter 5.

The modified LVM was extended into a third-order model capturing the competition between multiple fuel types. Other studies focus primarily on the introduction of hydrogen or other AFVs as single competing fuel type, however the main contribution from this chapter considers the penetration of both HBVs, NFC-EVs, and the impact on conventional vehicles. This enabled the analysis of the impact of both predators on conventional prey in addition to the impact of the two predators on each other. In this chapter, the HRS operating efficiency was also varied, analysing the impact on the number of HFCVs alongside using different penetration strategies with three competing vehicle types. Some recent studies have considered the variation of HRS efficiency, and this thesis contributed by allowing this by altering the parameter h. It is expected that the HRS will not operate at or near maximum capacity initially, assessing the impact of under-utilisation is important to gauge the impact of demand on the HRS network.

The final objective was addressed in chapter 6 where strategies were optimised with respect to fuel economy and emissions for the adoption of hydrogen in the UK's private vehicle fleet. The model was also optimised using LQR, where the LQR design is based on state feedback using all three variables. Six different scenarios were selected based on extreme, moderate, and best-case scenario for each vehicle type. The M1 model showed situations where both NFC-EVs and HBVs prospered. The M2 model enabled HBVs to attack both conventional and NFC-EVs. However, the number of NFC-EVs did not decline sharply or drastically. Both HBVs and NFC-EVs managed to acquire a significant proportion of the market share. Despite HBVs' attack on NFC-EVs, the ability to retain a similar level of figures suggest that the fuel input to the model has a larger bearing on the model. So, in other words, having the electrical infrastructure in place already from the national grid, it is easier for NFC-EVs to penetrate the private vehicle market and increase their proportion. The availability of supply chains and infrastructure is a critical component in determining the success of AFVs. The M3 model, showed two interesting simulations when the nine scenarios were simulated. In the case where both NFC-EVs and HBVs were on the best-case scenario (regardless of whether conventional vehicles were on extreme or moderate case scenarios), the NFC-EVs inhibited the growth of HBVs. The simulation graphs indicate that both showed an overshoot in the number of HBVs before settling below the expected number. Again, in real-life HBVs will compete with AFVs, and the vehicles with an established infrastructure and supply chains will become more prominent than HBVs, where new infrastructure is required. Having a greater fuel available whilst being allowed to attack and be attacked by HBVs seemed to give NFC-EVs an edge as shown in chapter 6.

Different scenarios were also simulated with a varying market share between NFC-EVs and HBVs, where the utilisation level of HRs were varied from 25, 50, 70, and 100%. The M3 model was used to simulate the different scenarios as it depicts reality as closely as possible. In all cases, it was difficult for HBVs to become dominant or fulfil the capacity available due to the current advantages of NFC-EVs. The maximise the efficiency is attained if the HRS network operates between 75-100%. By opting to use a dynamic model rather than static one, the evolution of conventional vehicles, and the impact of AFVs was considered over time. Further advantages compared to other models in literature include the model's strength, which demonstrates time reduction in simulating different scenarios and the significant reduction in computing power to achieve similar forecasts as other models as shown in chapter 6.

The last area of contributions lies in the direction and suggested insights of the modelling informing policymakers regarding the direction of the UK's passenger vehicle fleet planning from the case study. The case study highlighted that more than 50% market share could only be achieved by overcoming significant challenges and total focus on this sector. Since AFVs will also play a role, it was suggested that 50% market share should be used as the upper limit for further research and development. The optimum market share of hydrogen for the UK's private vehicle fleet is at 20% as shown in chapter 6.

Current emphasis is being placed on building small HRSs for the pre-commercialisation phase and while the demand for hydrogen is low. However, from this thesis, it is highlighted that larger HRS will be more beneficial in driving the towards a hydrogen economy. The excess hydrogen produced can be used in other sectors until the number of HBVs increases. Furthermore, it is also recommended that in the near-term, perhaps focusing on manufacturing HFC-REs over HFCVs will help to drive the attention towards hydrogen. The FC system can act as a range-extender to conventional vehicles or EVs. With EVs, it can prove to be an effective strategy for both vehicle types while increasing the range and reducing refuelling time as shown in chapter 6.

To conclude, this study indicates that the LVM based on growth concepts is a feasible tool to strategise and plan the Role of hydrogen in the UK's private fleet. However, there needs to be significant research efforts in exploring the role of hydrogen amongst other renewable transport fuels, and the source of this hydrogen. Further development of a centralised hydrogen network, alongside the electrical infrastructure will increase the overall prospects of hydrogen as a transport fuel.

7.3 Recommendations for further work

Different studies in the literature have used extensive modelling approaches to consider the penetration of hydrogen into the private vehicle market as a fuel. However, the adoption of hydrogen as a transport fuel for the private vehicle fleet is still in the initial stages of pre-commercialisation phase for the UK due to limited infrastructure, sustainable supply chains of hydrogen, and advancements in technology. The main hindrance for hydrogen, is the lack of governmental long-term planning and policies for its role and market share. Having a clear end goal for hydrogen will allow planning and execution of the strategy utilising the best route, instead of building initial small sized stations that can only provide hydrogen for a few vehicles. The best way forward is to have a continuous, and supportive policy framework to help integrate hydrogen as a fuel for the private fleet contributing to both national and international energy targets and emission cuts.

As a result, recommendations from this research study are as follows: -

- Implication to Practise

1) Significant research is required to identify the roles that each alternative fuel will play in the private fleet to ascertain the type of investment required in terms of the refuelling infrastructure, supply chains and vehicles. This will lead to long-term viability of a sustainable fleet, therefore positive impact on the environment and fuel security. This will then allow appropriate locations for the refuelling infrastructure, centralised production plants of different fuels maximising on efficiency and operation, and the optimum transportation modes for each.
2) For continuous application involving hydrogen as a transport fuel, the combined use of a centralised production network between different sectors would be recommended to identify the optimum use of the plant, avoiding under-utilisation periods, and covering periods of maximum output. The application of hydrogen in different sectors, or in niche/specific applications will enable cross use to minimise under-utilisation and improve the investment prospects.

3) The incorporation of the electrical components into the model in future work is essential to ascertain optimal infrastructure cost and the amount of fuel consumed in a HFC-RE.
4) To achieve favourable market for hydrogen, it is recommended that further research efforts should identify ways of shortening the supply chains of hydrogen especially using renewable energy means. To safeguard the use of hydrogen by allowing it to be used as an energy reserve for the national grid, whilst utilising the electricity to charge HFC-REs.
5) In order to optimise the strategy for HFCVs for the UK's private fleet, further studies should determine suitable locations for the centralised production near current pipeline networks for dual purpose use of hydrogen.
6) A framework is required to help to produce a standardisation of policies in terms of how effective they are in relation to other policies and the commitment of various stakeholders and governmental departments.
7) Further work is required in determining the impact of current legislations, and political sensitivities such as COVID-19 and warfare. Research and development are required in utilising and storing hydrogen as an energy reserve during these times.

- Implications to Policy

8) Finally, to ensure the hydrogen plays a role in decarbonising the UK's private fleet, a recommendation is to develop further policies incentivising hydrogen with stricter policies on emissions and pollution.

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Appendix A

Table A. 1:Table represents the results for different scenarios simulated for the M1 model at HRS operating at maximum capacities.

Scenarios	Conventional fuel input kg/year	ICEVs	NFC-EVs fuel input kg/year	NFC-EVs	Hydrogen Fuel input kg/year	HBVs
1	Impact on ICEVs		Extreme case		Extreme case	
	3.2e10	31.6e6	5.5e7	115400	1.46e6	8729
2	Impact on ICEVs		Moderate case		Extreme case	
	3.2e10	20.18e6	1e10	17.51e6	1.46e6	8176
3	Impact on ICEVs		Extreme case		Moderate case	
	3.2e10	20.83e6	5.5e7	112800	2e9	11.48e6
4	Impact on ICEVs		Best case		Extreme case	
	3.2e10	14.75e6	1.4e10	28.01e6	1.46e6	8063
5	Impact on ICEVs		Extreme case		Best case	
	3.2e10	24.97e6	5.5e7	106400	5e9	26.02e6
6	Impact on ICEVs		Moderate case		Moderate case	
	3.2e10	13.25e6	1e10	19.98e6	2e9	11.e6

Table A. 2: M2 model results

Scenarios	Conventional fuel input kg/year	ICEVs	NFC-EVs fuel input kg/year	NFC-EVs	Hydrogen Fuel input kg/year	HBVs
1	Impact on ICEVs		Extreme case		Extreme case	
	3.2e10	31.64e6	5.5e7	115400	1.46e6	9729
2	Impact on ICEVs		Moderate case		Extreme case	
	3.2e10	20.18e6	1e10	17.51e6	1.46e6	8176
3	Impact on ICEVs		Extreme case		Moderate case	
	3.2e10	20.84e6	5.5e7	96840	2e9	11.48e6
4	Impact on ICEVs		Best case		Extreme case	
	3.2e10	14.75e6	1.4e10	28.01e6	1.46e6	8063
5	Impact on ICEVs		Extreme case		Best case	
	3.2e10	24.98e6	5.5e7	32450	5e9	26.02e6
6	Impact on ICEVs		Moderate case		Moderate case	
	3.2e10	13.78e6	1e10	17.28e6	2e9	11.02e6

Table A. 3: M3 model results

Scenarios	Conventional fuel input kg/year	ICEVs	NFC-EVs fuel input kg/year	NFC-EVs	Hydrogen Fuel input kg/year	HBVs
1	Impact on ICEVs		Extreme case		Extreme case	
	3.2e10	31.64e6	5.5e7	115400	1.46e6	8125
2	Impact on ICEVs		Moderate case		Extreme case	
	3.2e10	20.18e6	1e10	17.52e6	1.46e6	455
3	Impact on ICEVs		Extreme case		Moderate case	
	3.2e10	21.23e6	5.5e7	97590	2e9	10.79e6
4	Impact on ICEVs		Best case		Extreme case	
	3.2e10	14.76e6	1.4e10	28.01e6	1.46e6	332
5	Impact on ICEVs		Extreme case		Best case	
	3.2e10	24.98e6	5.5e7	32450	5e9	26.02e9
6	Impact on ICEVs		Moderate case		Moderate case	
	3.2e10	17.23e6	1e10	19.93e6	2e9	630600

INTERNATIONAL JOURNAL OF HYDROGEN ENERGY 42 (2017) 24927–24938

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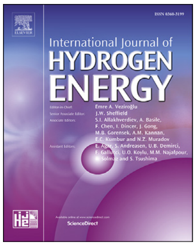

Review Article

Review of modelling approaches used in the HSC context for the UK

Sahdia Maryam

The Faculty of Computing, Engineering and the Built Environment Birmingham City University, United Kingdom

ARTICLE INFO

Article history:
Received 31 January 2017
Received in revised form
24 April 2017
Accepted 28 April 2017
Available online 7 September 2017

Keywords:
Hydrogen supply chains
Hydrogen infrastructure
Optimisation
GIS-based approaches
System dynamics

ABSTRACT

Hydrogen has an instrumental role to play in shaping the future of the UK's transport system. Huge reductions in ‘Greenhouse Gas’ (GHG) emissions may be achievable whilst providing a secure source of clean and sustainable fuel. Hydrogen transition has already begun but to strengthen and power the ‘hydrogen economy’ momentum in the UK, the development of the hydrogen infrastructure needs to make progress more quickly. There are many challenges associated with this due to the complexity at each node of Hydrogen Supply Chains (HSC), such as the number of processes to produce hydrogen. This raises the challenge to model HSCs, allowing analysis of various pathways and optimal configurations. This report aims firstly, to review the factors discussed in the literature on HSC and identify gaps or issues that require further debate with regards to introducing hydrogen in the transport system. Secondly, various HSC modelling techniques have been categorised according to mathematical methods used and the factors being considered. Studies in the literature have analysed hydrogen transport systems in terms of capital and operating costs of the infrastructure, and the cost of hydrogen, environmental implications and risk. A significant market share can be obtained by hydrogen in the near future with the minimisation of cost across the supply chain from production to end-use. Effective policies are required to speed up the process and increase the energy efficiency alongside mitigating GHGs and improving fuel security. Further developments in the mathematical optimisation models and technical breakthrough will enable the transition to a hydrogen economy take place with minimum disruption and issues.

Contents

E-mail address: sahdia.maryam@bcu.ac.uk.

http://dx.doi.org/10.1016/j.ijhydene.2017.04.303

Notation

CCF	Annual capital charge factor
FCC	Facility capital cost
FOC	Facility operating costs
GAMS	Generic algebraic modelling system environment
GIS	Geographical information systems
HFCV	Hydrogen Fuel Cell Vehicle
HSC	Hydrogen supply chain
ICV	Internal combustion engine vehicle
LCA	Lifecycle assessment
LCI_b	Life cycle inventory of chemical b
MILP	Mixed integer linear programming
NT	Number of time periods
PCA	Principal component analysis
PCC	Production capital cost
PEC	Production carbon emissions
PECC	Production energy consumption costs
POC	Production operating costs
POX	Partial Oxidation
PR_{igpt}	Production of hydrogen mode I via technology p in period t in location g
Q	expectation variable
QRA	Quantitative risk assessment method
$Q_{igg'Lt}$	Flow of hydrogen mode I via transportation mode l between locations g and g' in period t
SADM	spatially aggregated demand model
SCC	storage capital cost
SMR	Steam methane reforming
SMPM	Stochastic multi-periods model
SOC	Storage operating costs
TCC	Transportation capital cost
TDC	Total daily cost
TOC	Transportation operating costs
α	Network operating period
ω_b^{Pr}	Life cycle inventory of chemical b associate with hydrogen production
ω_b^{St}	Life cycle inventory of chemical b associated with hydrogen storage
ω_b^{Tr}	Life cycle inventory of chemical b associated with hydrogen transportation
ABM	Agent-based modelling
LVM	Lotka-Volterra model
BDM	Bass-diffusion model
SD	System Dynamics

Introduction

Hydrogen is emerging as one of the major energy carriers of the future energy system. Investing and building the hydrogen infrastructure has substantial risks especially with an uncertain demand [1]. For Hydrogen Fuel Cell Vehicles (HFCVs) or Internal Combustion Engines Vehicles (ICVs) using hydrogen as a fuel are to become a viable option then this issue needs to be addressed [2]. This paper will provide an overview of the Hydrogen supply chain (HSC) infrastructure and on current methods used to predict and optimise planning of a sustainable infrastructure.

The need for a transition to a hydrogen economy is being driven by the following factors; concern over climate change globally; the quality of air in major cities due to pollution; disastrous future impacts on the environment such as rising sea levels; having a secure and sustainable supply of energy; and increased consumption of energy worldwide since the industrial revolution [3,4]. Fig. 1 shows that consumption of energy from 1971 to 2012 has increased almost linearly. Maintaining this trend is unrealistic and depletion of fossil fuels are the key drivers to find alternative solutions to fuel our energy systems.

Using hydrogen alongside electricity as an energy carrier is an appropriate long-term option to reduce CO_2 emissions because of its abundance in the universe [5,6], and it can also act as a means of energy storage [7]. However, hydrogen does not exist alone in nature nor can it be produced directly, so therefore energy is consumed for its production before it can be delivered to the end-user via various pathways [4,8,9]. The advantage of using hydrogen is that it can be produced from all primary energy sources, such as, coal, natural gas, wind, solar and biomass energy [4,10–15], adding variety in production sources and methods, thus complicating the architecture of hydrogen supply chains whilst ensuring security of fuel supply [8].

The challenge is identifying the most suitable feedstock, production method, storage option, transportation mode and end use in terms of a number of factors such as cost, environment and production rate etc. For stakeholders to invest in developing the hydrogen infrastructure, there must be some certainty regarding payback and profit.

Hydrogen produced from renewable sources alone will not be able to match the volumes of global hydrogen requirements, but might yet meet the local demand. Hydrogen's renewable pathways currently reduce the CO_2 emissions, but are more costly. Hydrogen produced from fossil fuels is cheaper, despite including the cost of carbon capture and

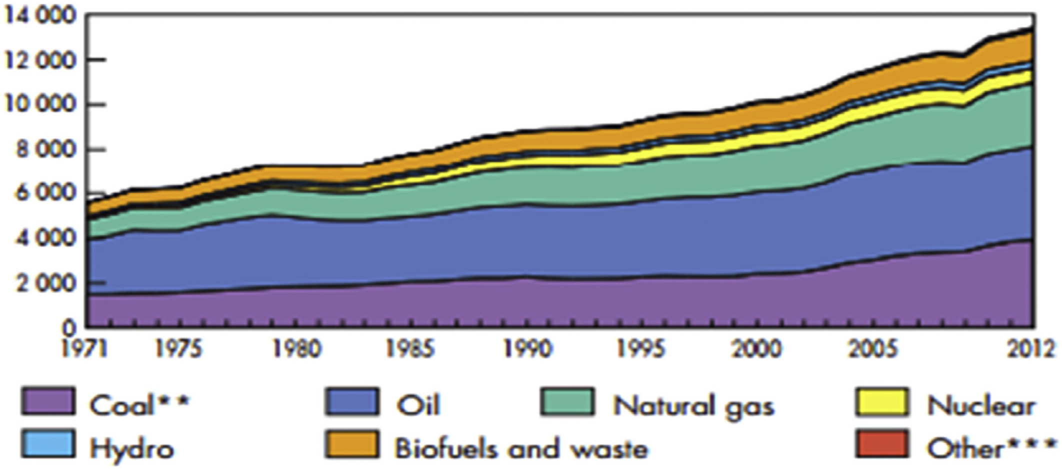

Fig. 1 – World total primary energy supply from 1971 to 2012 by fuel (Mtoe) [5].

storage (CCS) [15]. Further research and work is required to determine the hydrogen demand and then to find the most suitable means of meeting this demand.

Literature methodology

Research papers were identified and collated through the University's electronic journal databases and internet searches to search for papers using the following set of keywords: ‘Hydrogen’, ‘Hydrogen fuel cells’, ‘Hydrogen economy’, ‘Hydrogen Supply Chain’, ‘Hydrogen Infrastructure’. Some studies were also collated by using the author's name to see other papers written by them, while others were obtained by following the citations given. The electronic databases included sciencedirect.com; springer.com/; IEEE Xplore digital Library. Papers were mainly consulted between the period of 2005–2016 and papers were selected on the basis of using an optimisation or GIS-based approach, other papers were selected subject to the objective of the model. This paper primarily focuses on Mathematical models and Geographical Information System based models. The focus was to include studies specific to the UK but other models were also used. The initial review encompassed papers focusing on the HSC specifically and the secondary review included papers from SCs literature generally to fill in the gaps.

Literature review

The aim of this literature review is to identify the various approaches used by researchers to model the HSC. To classify the models according to the factors being considered such as cost. This will then develop the understanding of the most suitable approaches to model the HSC with regards to the important factors (objectives as chosen by the researcher). Developing an understanding what current papers have used as the objective of the models will help define what are the factors hindering the success of HFCVs and the implementation of the corresponding infrastructure.

Background of the hydrogen supply chains

The main obstacle hindering vehicle manufacturers and consumers from embracing HFCVs is the infrastructure, due to the complexity of infrastructure i.e. in terms of the options available at each node (e.g. production, distribution), which in turn have many options (e.g. renewable and non-renewable sources) [3,4,8,10,16]. Transitioning to a hydrogen economy can be achieved by overcoming the economic and technical issues [10] related to the infrastructure at each node of the HSC. Furthermore, the interactions between the nodes must also be analysed individually [8]. Constructing a new infrastructure will prove to be costly, and so the challenge is to acquire sufficient investment costs even though there is no assurance of a profitable demand. If a delivery infrastructure is developed, then this will fuel the implementation of HFCVs [3].

The methods of producing hydrogen are; Steam Methane Reformation (SMR), partial oxidation (POX) of fossil fuels, coal gasification, and water electrolysis [9,17], with thermochemical technologies to split water in early development [9]. In the case of storage, hydrogen can be stored as a gas, liquid, or nitrates [17,18]. Utilisation of hydrogen in Fuel Cells (FCs) offers more options over current fuels and emerging competitors especially for the transportation sector [10]. Hydrogen being the most abundant element in the universe simply changes state from water to hydrogen and vice versa during consumption [5,6], and is promising to become a major factor in speeding up the transition from the current energy system to a more sustainable energy system with low CO_2 emissions [11].

Review of optimisation approaches

HSCs are very complex to model so some researchers have chosen to use mathematical optimisation methods for this purpose. These approaches allow the optimisation of a complicated process, product, supply chain or some physical aspect with regards to a set of design variables, i.e. Cho and Kim [19] used optimisation methods to design and model a biomass-hydrogen pathway focusing on establishing efficient investment strategies. Optimisation models for the design and operation of HSCs may be steady state or dynamic; deterministic or Stochastic [1,20–22]. However, each model proposed in the literature is different with some aspects shared see Table 1 in Appendix 1. The main characteristic of optimisation models is that they tend to deal with the "how to" aspect of the problem rather than the "what if" aspect [8,23].

Mixed integer linear programming based approaches

Optimisation is a general automated design technique that enables the best optimal pathway or solution to be selected from a number of outcomes for a given problem. Mixed integer linear programming (MILP) is referred to when some of the variables are restricted to be integer [24]. Many researchers have chosen to base their model on MILP taking different design variables into account. The MILP models have been used to represent the HSC as a whole rather than each component separately with Almansoori and Shah leading the way [21].

MILP based models allow different parameters to be assessed as chosen by the researcher from determining the optimum infrastructural and operating costs to developing better understanding of the trade-offs in the HSC [21]. A number of cities and countries have been used as back-drops to models arriving at different conclusions about what the ideal pathway or hydrogen economy might look like [21,25]. This suggests that it is yet unclear as to what the hydrogen economy will look like and it is more likely that hydrogen pathways will be tailored according to the needs of each location.

The mathematical model developed by researchers will also impact the conclusions drawn, for instance, Almansoori and Shah [21] in their early work developed a model that only considered a 'snapshop' view of the future, whereas it is expected that the costs will vary according to the demand of hydrogen and the development of the infrastructure over time.

The main advantage of using MILP-based approaches is that they offer a flexible method to researchers investigating various objectives such as identification of the appropriate locations [26]; most economical pathway [27]; evaluation of the economic potential alongside the infrastructure requirements of a pathway for a certain location [28]; and to identify the least-cost pathway [29–31].

Multi-period model

Multi-period optimisation models generally have known parameters and different echelons are solved simultaneously. Furthermore, decisions and trade-offs can be made simultaneously between different periods. These models are generally considered to have a deterministic demand, however in recent literature stochastic demand has also been employed to make estimations of the probability distributions of potential outcomes by varying inputs over time.

Dayhim et al. [1] used a Stochastic Multi-Period Model (SMPM) to model the HSC network under uncertain demand detecting critical factors contributing to the design of an optimal network. Similarly, Almansoori and Shah [32] also developed a multi-period, MILP-based model taking uncertainty into account. While Almansoori and Shah [32] used a scenario-based approach to calculate uncertainty resulting from long-term variation in hydrogen demand. Dayhim et al. [1] used a Spatially Aggregated Demand Model (SADM) to estimate the potential demand for potential customers in purchasing HFCVs by considering household. Furthermore, the network described in the model is demand-driven. This implies that the production of hydrogen, and the development of storage facilities alongside the transportation links are directly proportional to the demand.

Hugo et al. [33] developed a generic optimisation-based model to strategically plan and develop a long-term investment design of future HSCs for HFCVs. MILP technique was utilised to find the optimal solutions concluding that the optimal SC design and investment strategy should instigate by utilising on-site, SMR of natural gas from the grid.

Li et al. [34] extended the previous work by Hugo et al. [33] using a generic optimisation-based model for the strategic-dynamic investment planning and design of the future HSCs using china as a case study. The model encompasses combines potential technologies within the HSC that are considered to be necessary in the strategic decision-making process to visualise the future HS infrastructure. The model identified optimal supply chain designs and eliminated inferior pathways, leaving the more promising ones.

A large study was conducted using a multi-period optimisation framework in the Netherlands [22] showing that the transition to a hydrogen-based transport is economically feasible on a large-scale, and can be used for any demand scenario. The resulting network was found to be similar to the existing gasoline infrastructure. Whereas Ren [35] assessed China's internal and external environment of hydrogen economy using a SWOT analysis before prioritising strategies promoting the hydrogen economy. Goal programming and fuzzy theory were integrated to form a multi-criteria decision making model. This enabled prioritisation between the effective strategies proposed, so that stakeholders can implement these strategies appropriately.

Multi-objective optimisation problem based models

Multi-objective optimisation problems look to simultaneously optimise more than one objective function. This approach is ideal where optimal decisions are required by making trade-offs between two or more conflicting objectives. This approach has been used in a number of studies in the HSC area, where authors have investigated the best solutions considering a number of variables such as cost, global warming and safety risk [22,34,36–40].

In contrast to MILP models mentioned previously, cost efficiency and safety were considered using a multi-objective optimisation approach, while demand uncertainty was assessed by analysing the deterministic and stochastic solutions [24,25,41,42]. A single objective with many constraints may not adequately represent the problem. Having more objectives will complicate the trade-offs and are less easily quantified [43].

Guillen-Gosalbez et al. [36] analysed the design of a HSC formulated as a bi-criterion MILP for vehicles considering economics and environmental impacts through a life-cycle analysis. Here, Almansoori and Shah's [21] model was extended, to encompass the progression of the network considering time-variant demand.

Multi-objective optimisation problems do not usually have a single optimum solution for the all the objectives simultaneously as the objectives are usually in conflict with each other e.g. reducing cost and the environmental impact. This results in a group of efficient solutions that fit the problem and a number of technique have been used by researchers to calculate the group of efficient points: aggregation of objectives, e-constraints, compromise programming etc. [44–47].

The development of HSC pathways is a necessary measure to analyse the behaviour of the energy system across the whole energy system. To achieve this, the models proposed need to give a precise account of the pathways linked with the techno-economic assumptions made. Furthermore, the models proposed in this section are static and SCs are often complicated and time-dependant, so therefore it is more likely that to accurately represent the HSC then a dynamic model must be proposed. Other types of optimisation models such as System Dynamics (SD) are perhaps a better at representing the interactions of a SC than linear modelling.

Review of geographical information system based approaches

The Geographical Information System (GIS) based approaches are an alternative method to model the HSC. These approaches are dependent on national or regional-specific conditions such as population, size, location, availability of resources etc. whereas optimisation approaches are more generic (see Table 2 in Appendix 1). Researchers have begun to use GIS packages more frequently and often include it as an element within a modelling system for SC management (SCM) [46] (see Tables 1 and 2).

A number of researchers have used an energy system optimisation framework to analyse long-term hydrogen fuel and vehicle adoption e.g. MARKAL/TIMES [48–51]. These frameworks enable the optimisation of the entire energy system so that competition for primary energy resources for the consideration of different energy services. Like optimisation approaches, there are many variants available with an important role to play within the energy system, further developments are required to enhance the analytical tools available to assess different aspects [52,53]. Utilising GIS, researchers have been able to identify possible hydrogen demand centres as well as supply locations and the infrastructure to link them. Some studies have combined GIS with other approaches such as mathematical optimisation methods [46,54], and heuristics algorithm [55]. These offer a more enhanced method to explore various aspects of the HSC.

The flexibility of GIS-based approaches allows a wide range of objectives and pathways to be analysed such as the design of the pipeline systems [54,56,57]; the location of hydrogen stations to fuel the flow of maximum number of vehicles [55], [58]; public acceptability [59]. Case studies have been conducted assessing various factors in specific regions such as Norway [60], Ohio [61], Southern California [62], Sweden [63], and Germany [64].

Transition models

This section includes other methodologies and approaches adopted by researchers to define and predict the transition to a hydrogen economy. Studies placed under this section aim to understand the behaviour of the HSC, under specific circumstances often including the projected costs of the various pathways, which can then be implemented on various scales from national or regional with location specific data.

Elgowainy [65] has suggested that the investment and operating costs of a refuelling station can be reduced by implementing an effective opening strategy. In other words, using tube-trailers initially will allow the station equipment to satisfy slightly higher demands. However, Mulder et al. [66] have shown that there isn't a clear winning pathway and the most suitable pathway must be determined according to the availability of resource, emissions, costs and energy demand.

Stephens-Romero et al. [67] used Preferred Combination Assessment (PCA) to model the estimation of emissions, GHGs and the energy efficiency of the HSC as a function of the technology mix on a life cycle, well to wheels (WTW) basis. In a different study [68], the authors used a comprehensive advanced planning methodology for the deployment of hydrogen infrastructure. They found that only 11%–14% of the number of hydrogen refuelling stations can provide comparable accessibility to drivers in a particular location compared to gasoline stations. However, Kang [69] found that the deviation time for HFCVs was not so different than the current reported travel deviation time after considering the deviation in travel patterns in order to refuel a HFCV at one of the 68 proposed stations for early adopters. Although early studies have shown that hydrogen refuelling time is promising, it remains questionable whether customer demand can be met on a sustained level.

Transition models have also been used to estimations on the hydrogen penetration scenarios for Europe [70], [71]; modelling and simulating current ideas amongst Dutch

Table 1 – Summary of mathematical optimisation approaches.

Mathematical optimisation approach	Characteristics	References
Mixed Integer Linear Programming (MILP)	All parameters are integers and fast to resolve. Reduced computing time and is a rigorous, flexible approach with extensive modelling capability.	[37,79]
Mixed integer non-linear Programming (MINLP)	Non-integer parameters are used and can be directly implemented in a modelling language. Increase in simulation time and are often complicated.	[79]
Multi-period problems (MPP)	All parameters are known and different echelons are solved simultaneously. Decisions and trade-offs can be made simultaneously between different periods. Can complicate the model.	[41]
Multi-objective problem (MOP)	Uncertain quantities, characterised by probability distributions. Different objective parameters can be analysed and traded-off. Can overly complicate the model.	[36,80]

Table 2 – Summary of the geographical information system approaches.

Type of model	Characteristics	Reference
GIS-based model	GIS – Geographical Information Systems environment. These rely on national or regional-specific information such as population, size, availability of resources etc., and can help identify specific conditions for different geographic scales.	[48,52,53,55]
Cluster strategy	Cluster Strategy – coordinated introduction of hydrogen vehicles and refuelling infrastructure in a few geographic areas.	[54]
MOREHyS (model for optimisation of regional hydrogen supply) model	MOREHys – a tool to assess the introduction of hydrogen as vehicle fuel by means of energy system analysis.	[56]
STREET (Spatially and Temporally Resolved Energy and Environment Tool)	STREET – systematic planning tool operating at the highest level of spatial detail and integrates multiple considerations.	[50]
Backwards Heuristics		[49]
GIS + Heuristics algorithm	Operations research (OR) models.	[47]
GIS-MARKAL (MARKet ALlocation)	MARKAL – a linear optimisation model. Its strength is in analysing resource competition in economic, engineering, environment and energy terms.	[43,45,81]
H2TIMES	H2TIMES – a quasi-spatial model.	[44]
MOP + ArcGIS	ArcGIS - A GIS used to organise, analyse and map spatial data.	[41]
Stochastic optimisation + GIS	Stochastic – a systematic search for optimal and near-optimal solutions.	[46]

stakeholders [72]; and to assess the impact of hydrogen on California's economy [73–75]; in Germany [76] where the impact of hydrogen for the near future was seen as negligible because of high investment costs; and in US [77] three approaches were discussed to estimate the number of stations required to enable convenient access to hydrogen fuelling.

System dynamic approaches

System dynamics (SD) studies the influence that policymaking has on system control including structural characteristics according to several unique factors in the methodology [78,79]. SD considers the dynamic behaviour of a system, in particular the changes in behaviour in relation to time. Furthermore, SD uses feedback structure to determine the origins of these dynamic changes. SD is often preferred in many disciplines, especially in innovation and new technologies because it overcomes the limitations of conventional statistical methods that primarily focus on correlations. Whereas, SD can analyse the inter-related relationship among multiple variables using simulations [80].

SD was used to assess the relationship of HFCVs and HR infrastructure by developing a large-scale model that encompassed various factors influencing the saturation of HFCVs using feedback loops [81]. However, this model was limited in terms of what each feedback loop demonstrated through proven theory or a well-known statistical method.

An insight showing the impacts that external variables have on HFCVs penetrating the market was assessed by the development of a generalised Bass diffusion model using SD [78]. Using, SD, allowed various factors to be assessed through the flexibility of the model in terms of the time taken to simulate and adopt changes in terms of the inputs. As a result, new demand models were produced analysing the penetration of HFCVs. Nevertheless, the model did not encompass a statistical analysis of feedback effects assessing the variation of potential adopters of HFCVs as a result of external factors, such as, a decrease in oil prices or vice versa.

Other types of models have also been used such as the dynamic GTAP model developed with LCA method to assess and project the development of the HSC and CO_2 emissions in Japan [82]. Similar models have also been proposed encompassing dynamic economic growth theory, including the behaviour of investors, growth of the population and capital stock accumulation [82,83].

Furthermore Agent-based modelling (ABM) has also been utilised in a number of studies to assess the interactions of individuals or groups on an autonomous system as a whole [84–87]. Huetink et al. [88] proposed an agent-based model to analyse the developmental process of HFCVs from niche to market utilising different strategies for the development of the infrastructure. Market penetration of HFCVs was also assessed using SC in the German market from different stakeholder perspectives [89]. The authors concluded that adequate support a third of all vehicles by 2040 could be propelled by hydrogen increasing to two-thirds by 2050.

Utilising SD to model the HSC opens up many exciting possibilities in integrating various tools and models to give alternative models to those discussed earlier. It is also possible to use models such as the Lotka-Volterra Model (LVM) to analyse the relationship between different types of vehicles and their introduction into the market.

Factors influencing the HSC decisions made

The following sections focus on what the literature is suggesting with regards to the important factors influencing the 'hydrogen economy'. Hydrogen is a driving force in the transition to a renewable energy based or low/zero emissions transport system. However, the hydrogen transition is being hindered by the lack of infrastructure, which is complicated due to the number of options available at each node.

From the literature, many researchers have pre-determined the pathway of the HSC for e.g. selecting the hydrogen production technology, type of storage and transportation mode before focusing on the objective of the model. Majority of the studies focused on mathematical optimisation approaches to determine the optimal configurations of the HSC. Several important factors (objectives of the model) have been outlined from the literature review, and prioritising these is critical in selecting the most optimal HSC for the UK. The most prominent factor being cost. Several studies focus on minimising the cost across the HSC, whereas others focus on minimising the environmental impact. Reducing the risk factor of investing in building the hydrogen infrastructure in terms of investment as well as supply disruption are also critical to make it a promising adventure for investors. Cost, and environmental factors have been critical in defining the design of the HSC.

Minimisation of cost

One of the challenges faced by various stakeholders is the cost of implementing the hydrogen infrastructure, and many studies have focused primarily on minimising the cost across the HSC [1,25,27,29,37]. The total cost (see Eqs. (1)–(3)) includes both the capital and operating costs of the HSC. The capital costs encompasses the one-off costs associated with establishing the production plants, storage facilities and the transportation modes, whereas the operating costs encompasses the costs incurred on a daily basis such as the operation of production plants [21,25].

$$TDC = \frac{FCC + TCC}{\alpha CCF} + FOC + TOC \tag{1}$$

The total daily cost of the HSC (TDC) is formulated by taking a number of factors into account such as facility capital cost (FCC), transportation capital cost (TCC), facility operating cost (FOC), total transportation operating cost (TOC), annual capital charge factor (CCF), product operating costs (POC), production capital cost (PCC), storage capital cost (SCC), and the network operating period (α). Eg.1 represents the deterministic solutions to obtain the TDC, whereas Eq. (2) takes demand uncertainty into account by analysing the deterministic and stochastic solutions [25].

$$TDC = \frac{1}{\alpha CCF}(PCC + SCC) + POC + E_{\xi}\left[\frac{TCC_{\xi}}{\alpha CCF} + SOC_{\xi} + TOC_{\xi}\right] \tag{2}$$

To calculate the overall cost, then hydrogen demand must be determined. The hydrogen demand has been estimated through a number of models [1,7,32,56,90,91], considering various factors such as household income, households with more than one vehicle, education, commute distance, number of HFCVs, penetration factor of HFCVs, population density etc.

Fluctuations in hydrogen demand will influence the cost due to inefficient use of hydrogen plants or the need to construct new power transfer lines to manage the increase of energy. Dayhim et al. [1] expanded the previous work done and developed a multi-period two-stage stochastic model under demand uncertainty to minimise the total social cost (TSC) (Eq. (3)). The model developed is capable of running many scenarios with probabilities that are defined by the user. The equation developed takes various variables into account such as emissions, consumption and risk costs [1].

$$Min\ TSC = \frac{1}{NT}\left(\frac{1}{\alpha CCF}(PCC + SCC) + POC + PEC + PECC + PRC + Q\right) \tag{3}$$

where PCC = production capital cost; PEC production carbon emissions; production energy consumption cost = PECC; production risk cost = PRC, and expectation variable = Q.

Further developments and reductions in hydrogen production and storage technologies alongside cost-competitive transportation will reduce the costs incurred for implementing the hydrogen infrastructure. More research must be focused on hydrogen production to deliver lower costs and more sustainable fuel flow.

Reducing the environmental impacts

Reducing the impact that road transportation has on the environment is a driving force to introduce low or zero emissions vehicles. While HFCV is a zero emissions vehicle at the point of end-use, emissions are incurred during the production, transportation and storage nodes. These can be reduced by using clean feedstock to produce hydrogen and further developments in technology. Using CCS will mitigate CO_2 emissions, but will increase the cost.

The environmental impact of transitioning to a hydrogen economy has been analysed using the Life-cycle Analysis (LCA) or inventory (LCI) approaches by researchers as in the case of Miotti et al. (2017) [78] who conducted a LCA to assess the current state of hydrogen FC technology. LCA can be used to measure the environmental benefit of adopting the HSC [36]; evaluate the CO_2 emissions relative to production, storage and transportation [37,39]; evaluate the emission and feedstock requirements to calculate the environmental impact of the HSC [38]; and to evaluate the environmental aspects in relation to the production, distribution and storage of hydrogen [38,92].

$$LCI_b = \sum_i \sum_g \sum_p \sum_t PR_{igpt}\left(\omega_b^{Pr} + \omega_b^{St}\right) + \sum_i \sum_g \sum_{g' \neq g} \sum_{i \Delta IL(l)} \times \sum_t Q_{igg'Lt}\,\omega_b^{Tr}\ \Delta b \tag{4}$$

where ω_b^{Pr}, ω_b^{St} *and* ω_b^{Tr} denote the LCI entries (i.e. defined by the user e.g. emissions related to the environment) associated with chemical b per reference flow of activity [38].

The LCI can be expressed as a function of the production rates at the plants (PR_{igpt}), and hydrogen flows ($Q_{igg'Lt}$). The first term in Eq. (4) represents the emissions linked with the manufacture and storage of hydrogen, whereas the second term relates to the emissions associated with the transportation of hydrogen between sub-regions.

The global hydrogen pathway will face the complication to compromise between vital criteria such as minimising both cost and emissions. Economical pathways will not necessarily correlate to the ideal green pathways.

Hydrogen options

The studies reviewed are inconclusive with regards to the most appropriate pathway or steps for the UK to undertake in its journey to achieving its 2050 transport decarbonising targets. It is more likely that localised small-scale hydrogen production will suffice initially, perhaps from chemical processing plants or on-site production until the demand increases. Furthermore, the technique used to produce hydrogen will play a promising role in determining the timescale of when the hydrogen infrastructure will be installed. However, it is clear that no single hydrogen production method will be sufficient to produce enough hydrogen to fulfil the expected demand on its own.

From the hydrogen production options available, SMR is the cheapest while producing the least CO_2 emissions compared to the rest. The second most attractive option is coal gasification, which when utilised with CCS is both economically and environmentally attractive. For remote locations, water electrolysis is the most attractive option. It is inevitable that hydrogen will be produced on-site initially and localised production technologies such as electrolysis will play a crucial role in introducing hydrogen for early market adoption and low populations. However, introducing hydrogen into high populous areas will reduce the infrastructure costs with on-site production reducing distribution costs in contrast to centralised production. As hydrogen demand increases, incremental capacity can be added to increase the capacity as required. This will help keep costs low with the uptake of HFCVs increasing.

Liquefied hydrogen is most economic using large power plants and with dispersed hydrogen demand [64]. Hydrogen produced from renewable energy will be a crucial role in reducing global warming impacts and fuel consumptions [63,92], alongside transportation of hydrogen to it [44,45]. Availability of biomass for hydrogen production alongside CCS are also critical in achieving low costs and emissions [49]. But hydrogen from non-renewables is expected to dominate initially because of cost and infrastructure being in place already. Policies and CO_2 targets will help the transition from fossil-based hydrogen to green hydrogen. Furthermore, cost reductions in renewable technology achieved by mass production, feedstock costs and availability will strongly influence the cost of green hydrogen.

Large power plants are not required initially due to high costs in transporting the fuel to the required locations [93], however centralised production plants are an ideal route to the hydrogen economy [32] and perhaps ideal at low market penetration [61]. Industrialised hydrogen will also play a role in initiating the transition to a hydrogen economy with onsite SMR supporting the demand before moving to more centralised production [27].

In terms of distribution, huge investments are required before a sizeable infrastructure is in place to maintain the demand expected. There are many options available to transport hydrogen depending on the volume of hydrogen, delivery distances etc. compressed gaseous and liquid hydrogen can be distributed by trucks and rail with gaseous hydrogen through a pipeline infrastructure. However, the cost of building a centralised infrastructure for distribution such as pipelines has high capital costs [70]. A localised distribution infrastructure will initiate and maintain the hydrogen local hydrogen until it is seen viable and profitable before governments and stakeholders will invest in a more centralised infrastructure. Investing in a pipeline distribution is ideal for low market penetration [61], while truck and rail delivery will offer a competitive option in the UK [21,32].

Having an adequate refuelling infrastructure in place alongside the deployment of HFCVs in the market will meet the expectations of potential customers. The hydrogen infrastructure required is expected to be similar to the current infrastructure [22] where customers can expect the deviation time to be similar to the current reported time in order to refuel a HFCV at one of the proposed 68 stations [69]. However, in a different study it was found that only 11–14% of the hydrogen refuelling stations can provide comparable accessibility to drivers compared to gasoline [68]. Introducing hydrogen in clusters is the most effective strategy for an efficient design [55,62], as this and longer vehicle ranges will reduce the need of having many refuelling stations [26].

From the literature, it can be determined that initially the infrastructure will have to be developed alongside HFCVs in the UK, and most likely with the involvement of the vehicles manufacturers themselves. Once the number of HFCVs on the road increases, then more investment into the infrastructure will become necessary exceeding the rate of HFCV growth. Both, renewable and non-renewable energy sources will be utilised until sufficient renewable plants are in place to accommodate the hydrogen demand. So, therefore, beyond the initial period, the growth rate of infrastructure will have to be significant to attain long-term sustainability in the UK's road transport network.

Challenges influencing the design of the HSC

The transition to a hydrogen economy is happening due to it being a promising alternative for current transportation fuel. Reducing the cost of hydrogen across the supply chain will play a direct role in gaining market share. To aid this development, effective policies are required to speed up the process and increase the energy efficiency alongside mitigating GHGs and improving fuel security. Further support is needed from governments and this must also be included in the models.

Further research is required to generate new perceptions of hydrogen demand market, which will further the understanding of the future hydrogen infrastructure. The following aspects must be taken considered:

1) Contributions from utility companies, vehicle manufacturers and other stakeholders will have an impact on hydrogen demand, hydrogen produced, and the cost of production.
2) Further research is required in the area of utilising alternative and clean feedstock for the hydrogen production, and the corresponding pathways. More work needs to be undertaken on the technical aspects related to operating a HSC.
3) Furthermore, reducing the uncertainties regarding a hydrogen future, then commercialisation of hydrogen from the view-point of HSC needs to be undertaken.
4) Further development in HSC models utilising alternative models from the wider SC literature, equipment, technical breakthroughs alongside other technical standards are required to ensure the transition does take place with minimum disruption and issues. These developments are causing challenges for the commercialisation of hydrogen.
5) In terms of GIS-based approaches, current gaps are associated with the spatial distribution of hydrogen production and refuelling stations. It is more likely that GIS will be included as a component of an optimisation method to provide the best overview of the future hydrogen infrastructure.

A wide spectrum of hydrogen futures/pathways have been mentioned in the literature and it is not yet clear how the hydrogen economy will look like. However, there is consensus in the literature indicating that localised hydrogen will be used in highly populous areas initially before expanding to less populous areas forming a more decentralised network for which inter-connected sub models may be developed. The modelling will assume that all current pathways are available to calculate hydrogen demand and storage. It is more likely that the transition to a hydrogen economy will start off slow and then speed up as the number of stakeholders involved increases alongside the number of HFCVs.

Conclusion

The objective was to classify various approaches according to the type of method used to design the HSC. A review of the current approaches was proposed in the literature review to plan how the future HSC will look like. The literature review has identified a number of categories where most of the models have focused on mathematical optimisation including the MILP, stochastic multi-period, and multi-objective optimisation problem based. These models are most effective in addressing the question of future hydrogen infrastructure design enabling generalised formulation of the future HSC and may be applied to various case studies. However, they are static models only limiting the behaviour of the HSC to a snapshot or to very particular scenarios. Most of the studies have focused on cost, environmental and risk factors, but further work needs to be done to encompass other variables such as clean feedstock, technical feasibility, and performance of a renewable HSC alongside these factors.

The research presented in this article did not receive any specific grant from funding agencies in the public, commercial, or not-for-profit.

Appendix

Table A.1 – Summary of mathematical optimisation approaches covered in the review.

Mathematical optimisation approach	Characteristics	References
Mixed Integer linear programming (MILP)	All parameters are integers and fast to resolve. Reduced computing time and is a rigorous, flexible approach with extensive modelling capability.	[42,94]
Mixed integer non-linear Programming (MINLP)	Non-integer parameters are used and can be directly implemented in a modelling language. Increase in simulation time and are often complicated.	[94]
Multi-period problems (MPP)	All parameters are known and different echelons are solved simultaneously. Decisions and trade-offs can be made simultaneously between different periods. Can complicate the model.	[46]
Multi-objective problem (MOP)	Uncertain quantities, characterised by probability distributions. Different objective parameters can be analysed and traded-off. Can overly complicate the model.	[41,40]

Table A.2 – Summary of the geographical information system approaches covered in the review.

Type of Model	Characteristics	Reference
GIS-based model	GIS – Geographical Information Systems environment. These rely on national or regional-specific information such as population, size, availability of resources etc., and can help identify specific conditions for different geographic scales.	[56,60,61,63]
Cluster strategy	Cluster Strategy – coordinated introduction of hydrogen vehicles and refuelling infrastructure in a few geographic areas.	[62]
MOREHyS (model for optimisation of regional hydrogen supply) model	MOREHys – a tool to assess the introduction of hydrogen as vehicle fuel by means of energy system analysis.	[64]
STREET (Spatially and Temporally Resolved Energy and Environment Tool)	STREET – systematic planning tool operating at the highest level of spatial detail and integrates multiple considerations.	[58]
Backwards heuristics		[57]
GIS + Heuristics algorithm	Operations research (OR) models.	[55]
GIS-MARKAL (MARKet ALlocation)	MARKAL – a linear optimisation model. Its strength is in analysing resource competition in economic, engineering, environment and energy terms.	[48,50,95]
H2TIMES	H2TIMES – a quasi-spatial model.	[49]
MOP + ArcGIS	ArcGIS - A GIS used to organise, analyse and map spatial data.	[46]
Stochastic optimisation + GIS	Stochastic – a systematic search for optimal and near-optimal solutions.	[54]

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